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FILE COVERS 1907 - 27 Jun 2007  VOL 147 ISS 1
FILE LAST UPDATED: 26 Jun 2007  (20070626/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE


=> d stat que L23
L1              STR
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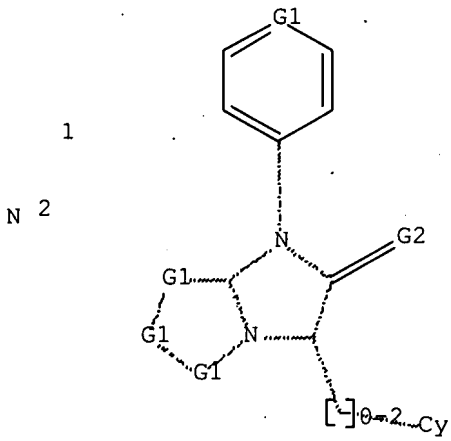

G1 [@1],[@2]
G2 O,S

Structure attributes must be viewed using STN Express query preparation:
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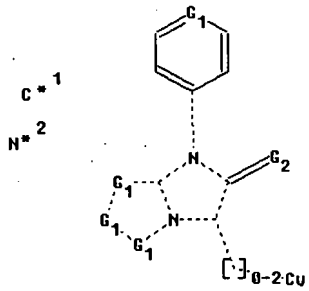

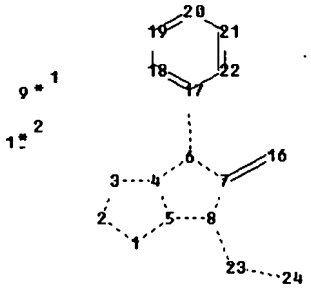

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16 23 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22
chain bonds :
6-17 7-16 8-23 23-24
ring bonds :
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exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 6-17 7-8 7-16 8-23 17-18 17-22 18-19
19-20 20-21 21-22 23-24

G1:[*1],[*2]

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom
Generic attributes :
24:
Saturation : Unsaturated

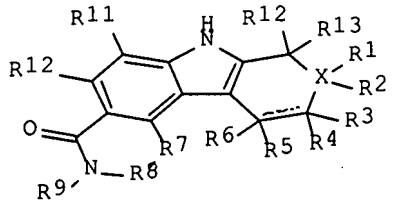
L4	22734	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	WU J?/AU
L5	1187	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	KELLY T?/AU
L6	419	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	LEMIEUX R?/AU
L7	1095	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	GOLDBERG D?/AU
L8	8	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	EMEIGH J?/AU
L9	21	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	SORCEK R?/AU
L10	16	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L4 AND (L5 OR L6 OR L7 OR L8 OR L9)
L11	11	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L5 AND (L6 OR L7 OR L8 OR L9)
L12	2	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L6 AND (L7 OR L8 OR L9)
L13	2	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L7 AND (L8 OR L9)
L14	3	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L8 AND L9
L15	22	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	(L10 OR L11 OR L12 OR L13 OR L14)
L19	572	SEA FILE=REGISTRY SSS FUL L1		
L20	28	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L19
L22	7	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	(L4 OR L5 OR L6 OR L7 OR L8 OR L9) AND L20
L23	23	SEA FILE=ZCAPLUS ABB=ON	PLU=ON	L15 OR L22

=> d ibib abs hitind L23 1-23

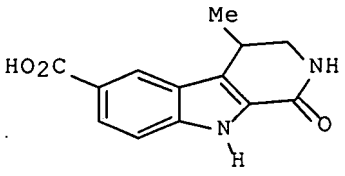
L23 ANSWER 1 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1286266 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:45497
TITLE: Anti-cytokine heterocyclic compounds as MAPKAP-K2 inhibitors and their preparation, pharmaceutical compositions and use in the treatment of diseases
INVENTOR(S): ***Goldberg, Daniel***; Abeywardane, Asitha; Miller, Craig; Morwick, Tina; Netherton, Matthew; Snow, Roger; Wang, Ji; ***Wu, Jiang-Ping***; Xiong, Zhaoming
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 82pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2006276496	A1	20061207	US 2006-276933		20060317
PRIORITY APPLN. INFO.:			US 2005-662936P	P	20050317
			US 2005-719164P	P	20050921

OTHER SOURCE(S): MARPAT 146:45497
GI



I



II

AB Heterocyclic compds. of formula I and analogs thereof and their use as inhibitors of Mitogen-Activated Protein Kinase-Activated Protein kinase-2 (MAPKAP-k2), and also to a method for preventing or treating a disease or disorder that can be treated or prevented by modulating the activity of MAPKAP-K2 in a subject and to pharmaceutical compns. and kits that include these MAPKAP-K2 inhibitors. Compds. of formula I wherein X is C and N; R1 is H, OH, carbamoyl, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R2 is absent, H, OH, ureido, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R3 is H, amino, C1-6 alkyl(amino), C2-6 alkenyl(oxy), C2-6 alkynyloxy, C1-6 alkynyl, etc.; R4 is absent, H, amino, C1-6 alkyl(amino), C2-6 alkenyl, CN, C1-6 alkynyl, etc.; R5 is absent, H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, OH, etc.; R6 is H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), oH, C3-7 cycloalkyl, etc.; R7 is H, C1-6 alkyl, C3-7 cycloalkyl, C1-6 alkoxy, OH, etc.; R8 is H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, and C3-7 cycloalkyl; R9 us H, halo, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R10 and R11 are independently H, C1-6 alkoxy, OH, halo, C1-6 alkyl, and C3-7 cycloalkyl; R12 is =S, =O, C1-6 alkyl, CN, aminoalkyl, amino, haloalkyl, etc.; R13 is absent, H, C1-6 alkyl, and halo; and their pharmaceutically acceptable salts are claimed. Example compound II was prepared by conjugate addition of di-Et malonate to methacrylonitrile; the resulting 2-(2-cyano-2-methylethyl)malonic acid di-Et ester underwent cyclization to give 5-methyl-2-oxopiperidine-3-carboxylic acid Et ester, which underwent condensation with sodium nitrite and 4-aminobenzoic acid Et ester to give 4-[N'-(5-methyl-2-oxopiperidin-3-ylidene)hydrazino]benzoic acid Et ester, which underwent cyclization to give 4-methyl-1-oxo-2,3,4,9-tetrahydro-1H- β-carboline-6-carboxylic acid Et ester, which underwent hydrolysis to give compound II. All the invention compds. were evaluated or their MAPKAP-K2 inhibitory activity.

INCL 514291000; 514411000; 548444000; 546085000
CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L23 ANSWER 2 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1286238 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:45542
TITLE: Anti-cytokine heterocyclic compounds as MAPKAP-K2

inhibitors and their preparation, pharmaceutical compositions and use in the treatment of diseases

INVENTOR(S): ***Goldberg, Daniel***; Abeywardane, Asitha; Miller, Craig; Morwick, Tina; Netherton, Matthew; Snow, Roger; Wang, Ji; ***Wu, Jiang-Ping***; Xiong, Zhaoming

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 50pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

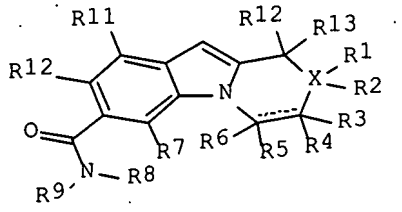
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2006276453	A1	20061207	US 2006-276935		20060317
PRIORITY APPLN. INFO.:			US 2005-662567P	P	20050317
			US 2005-719017P	P	20050921

OTHER SOURCE(S): MARPAT 146:45542

GI



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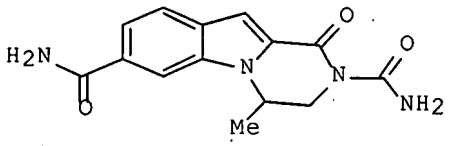

II

AB Heterocyclic compds. of formula I and analogs thereof and their use as inhibitors of Mitogen-Activated Protein Kinase-Activated Protein kinase-2 (MAPKAP-k2), and also to a method for preventing or treating a disease or disorder that can be treated or prevented by modulating the activity of MAPKAP-K2 in a subject and to pharmaceutical compns. and kits that include these MAPKAP-K2 inhibitors. Compds. of formula I wherein X is C and N; R1 is H, OH, carbamoyl, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R2 is absent, H, OH, ureido, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R3 is H, amino, C1-6 alkyl(amino), C2-6 alkenyl(oxy), C2-6 alkynyloxy, C1-6 alkynyl, etc.; R4 is absent, H, amino, C1-6 alkyl(amino), C2-6 alkenyl, CN, C1-6 alkynyl, etc.; R5 is absent, H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, OH, etc.; R6 is H, oxo, C1-6 (halo)alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), OH, C3-7 cycloalkyl, etc.; R7 is H, C1-6 alkyl, C3-7 cycloalkyl, C1-6 alkoxy, OH, etc.; R8 is H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, and C3-7 cycloalkyl; R9 us H, halo, C1-6 alkyl, C2-6 alkenyl(oxy), C2-6 alkynyl(oxy), C1-6 alkoxy, etc.; R10 and R11 are independently H, C1-6 alkoxy, OH, halo, C1-

6 alkyl, and C3-7 cycloalkyl; R12 is =S, =O, C1-6 alkyl, CN, aminoalkyl, amino, haloalkyl, etc.; R13 is absent, H, C1-6 alkyl, and halo; and their pharmaceutically acceptable salts are claimed. Example compound II was prepared by amidation of 4-methyl-1-oxo-1,2,3,4-tetrahydropyrazino[1,2-a]indole-7-carboxylic acid followed by carbamoylation with Ghosez's reagent. All the invention compds. were evaluated or their MAPKAP-K2 inhibitory activity.

INCL 514214010; 514220000; 514250000; 514291000; 544344000; 540558000; 540586000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L23 ANSWER 3 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1225839 ZCAPLUS Full-text

DOCUMENT NUMBER: 146:7960

TITLE: Derivatives of 6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonic acid and their preparation, pharmaceutical compositions, and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases

INVENTOR(S): Barry, John Patrick; Eriksson, Magnus Carl Arne; Joseph, David P.; ***Lemieux, Rene' Marc***; Wang, Xiao-Jun

PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany

SOURCE: U.S. Pat. Appl. Publ., 30pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006264472	A1	20061123	US 2006-382940	20060512
WO 2007027233	A2	20070308	WO 2006-US16903	20060503
WO 2007027233	A3	20070426		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-682462P P 20050519

OTHER SOURCE(S): MARPAT 146:7960

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Derivs. of 6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonic acid of formula I, which exhibit good inhibitory effect upon the interaction of CAMs and Leukointegrins and are thus useful in the treatment of inflammatory disease.

Compds. of formula I wherein R1 is OH and NH2; R2 is (un)substituted pyridinyl, (un)substituted pyrimidinyl, CN, halo, NH2 and derivs., and OCF3; R3 is (un)branched C1-3 alkyl; each R4 are independently halo, C1-2 haloalkyl; X is CH=, N=; Y is O and S; and their pharmaceutically acceptable salts thereof are claimed. Example compound II was prepared by iodination of (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-3- methyl-1H-imidazo[1,2-a]imidazol-2-one followed by sulfonylation; the resulting imidazo[1,2-a]imidazolesulfonyl chloride underwent hydrolysis to give the corresponding (4-bromobenzyl)imidazo[1,2-a]imidazole-3-sulfonic acid, which underwent boration with bispinacloato diboron to give the corresponding arylborate which underwent cross coupling with 4-amino-5-bromopyrimidine to give compound II. All the invention compds. were evaluated for their inhibition of LFA-1 binding to ICAM-1. From the assay, it was determined that the tested compds. exhibited Kd values of < 10 μM.

INCL 514338000; 514393000; 546273100; 548303100

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT ***915385-21-6P 915385-22-7P 915385-23-8P***
915385-24-9P 915385-25-0P 915385-26-1P
915385-30-7P 915385-31-8P 915385-32-9P
915385-33-0P 915385-34-1P 915385-35-2P
915385-36-3P 915385-37-4P 915385-38-5P
915385-39-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dihydroimidazoimidazolesulfonic acid derivs. and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases)

IT 1439-10-7, 4-Amino-5-bromopyrimidine 73183-34-3 ***321656-72-8***
688756-17-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dihydroimidazoimidazolesulfonic acid derivs. and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases)

IT ***321657-06-1P 321657-07-2P 321719-03-3P***
321721-20-4P 321724-08-7P 688756-08-3P
688756-18-5P 688756-19-6P 915385-27-2P
915385-28-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dihydroimidazoimidazolesulfonic acid derivs. and their inhibitory activity upon interaction of CAMs and leukointegrins and use in the treatment of inflammatory diseases)

L23 ANSWER 4 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:357148 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:39831
TITLE: Evolution of the Thienopyridine Class of Inhibitors of IκB Kinase-β: Part I: Hit-to-Lead Strategies
AUTHOR(S): Morwick, Tina; Berry, Angela; Brickwood, Janice; Cardozo, Mario; Catron, Katrina; DeTuri, Molly; ***Emeigh, Jonathan***; Homon, Carol; Hrapchak, Matt; Jacober, Stephen; Jakes, Scott; Kaplita, Paul; ***Kelly, Terence A.***; Ksiazek, John; Liuzzi, Michel; Magolda, Ronald; Mao, Can; Marshall, Daniel; McNeil, Daniel; Prokopowicz, Anthony, III; Sarko, Christopher; Scouten, Erika; Sledziona, Cynthia; Sun, Sanxing; Watrous, Jane; ***Wu, Jiang Ping***;

Cywin, Charles L.
CORPORATE SOURCE: Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT, 06801-0368, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(10), 2898-2908
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:39831

AB High-throughput screening is routinely employed as a method for the identification of novel hit structures. Large nos. of active compds. are typically procured in this way and must undergo a rigorous validation process. This process is described in detail for a collection of screening hits identified as inhibitors of IκB kinase-β (IKKβ), a key regulatory enzyme in the nuclear factor-κB (NF-κB) pathway. From these studies, a promising hit series was selected. Subsequent lead generation activities included the development of a pharmacophore hypothesis and structure-activity relationship (SAR) for the hit series. This led to the exploration of related scaffolds offering addnl. opportunities, and the various structural classes were comparatively evaluated for enzyme inhibition, selectivity, and drug-like properties. A novel lead series of thienopyridines was thereby established, and this series advanced into lead optimization for further development.

CC 1-3 (Pharmacology)
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:229064 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:343275
TITLE: An orally active, primate selective antagonist of LFA-1 inhibits delayed-type hypersensitivity in a humanized-mouse model
AUTHOR(S): Panzenbeck, Maret J.; Jeanfavre, Deborah D.; ***Kelly, Terence A.; Lemieux, Rene;*** Nabozny, Gerald; Reilly, Patricia L.; Desai, Sudha
CORPORATE SOURCE: Department of Immunology and Inflammation, Boehringer Ingelheim Pharmaceutical Inc., Ridgefield, CT, 06877-0368, USA
SOURCE: European Journal of Pharmacology (2006), 534(1-3), 233-240
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Compound I, a novel small mol. antagonist (Kd = 6 nM) of human lymphocyte function-associated antigen-1 (LFA-1, CD11a/CD18) was tested for activity in a humanized mouse model of delayed-type hypersensitivity (trans vivo delayed-type hypersensitivity). Trans vivo delayed-type hypersensitivity is a model for testing compds. with human targets in mice. Tetanus toxoid and 7-10 + 106 human peripheral blood mononuclear cells from tetanus-sensitized donors were coinjected into footpads of naive mice. Footpads were measured before and 24 h later. Injection of peripheral blood mononuclear cells plus antigen resulted in swelling of 0.178-0.254 mm, significantly greater than peripheral blood mononuclear cells or tetanus toxoid alone ($P < 0.05$). Preincubation of peripheral blood mononuclear cells with anti-human major histocompatibility complex class II (MHCII) or anti-human LFA-1 monoclonal antibody (mAb), but not anti-mouse MHCII or anti-mouse LFA-1 mAb, significantly inhibited the response. Compound I inhibited footpad swelling in a dose related manner (0.1-100 mg/kg, p.o.; ED50 .apprx. 1 mg/kg), whereas its enantiomer had no

effect. These data demonstrate the oral efficacy of a novel antagonist of LFA-1 in trans vivo delayed-type hypersensitivity.

CC 1-7 (Pharmacology)

IT ***321656-63-7***
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(LFA-1 antagonist activity in delayed-type hypersensitivity)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 6 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:168805 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:410694
TITLE: Alkylation of Magnesium Sulfinates: A Direct Transformation of Functionalized Aromatic/Heteroaromatic Halides into Sulfones
AUTHOR(S): ***Wu, Jiang-Ping; Emeigh, Jonathan;*** Su, Xi-Ping
CORPORATE SOURCE: Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA
SOURCE: Organic Letters (2005), 7(7), 1223-1225
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:410694

AB Sulfinate alkylation is one of the conventional methods for sulfone synthesis. The alkylation of magnesium sulfinates, which are easily accessible via reactions of organomagnesium intermediates with sulfur dioxide, provides a convenient route for sulfone preparation In this communication, the authors report a preliminary study of the alkylation of arylmagnesium sulfinates. An application of this reaction to directly transform functionalized aromatic/heteroarom. halides into sulfones is also described.

CC 21-2 (General Organic Chemistry)

IT 96-33-3, Methyl acrylate 922-67-8, Methyl propiolate 1120-90-7, 3-Iodopyridine 1521-51-3 4753-59-7 7446-09-5, Sulfur dioxide, reactions 16494-36-3 33240-34-5, Cyclopentylmagnesium bromide 40596-44-9 51934-41-9, Ethyl 4-iodobenzoate ***321656-73-9*** 850425-82-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of sulfones via generation of Grignard reagents from aromatic/heteroarom. halides by magnesium-halide exchange followed by reaction with sulfur dioxide and alkylation of the magnesium sulfinate intermediates)

IT ***321723-77-7P*** 850425-75-1P 850425-76-2P 850425-77-3P 850425-78-4P 850425-81-9P 850425-83-1P 850425-84-2P 850425-85-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of sulfones via generation of Grignard reagents from aromatic/heteroarom. halides by magnesium-halide exchange followed by reaction with sulfur dioxide and alkylation of the magnesium sulfinate intermediates)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:790832 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:6469
TITLE: Second-generation lymphocyte function-associated antigen-1 inhibitors: 1H-imidazo[1,2-α]imidazol-2-one derivatives

AUTHOR(S): ***Emeigh, Jonathan***; Gao, Donghong A.; ***Goldberg, Daniel R.***; Kuzmich, Daniel; Miao, Clara; Potocki, Ian; Qian, Kevin C.; ***Sorcek, Ronald J.***; Jeanfavre, Deborah D.; Kishimoto, Kei; Mainolfi, Elizabeth A.; Nabozny, Gerald, Jr.; Reilly, Patricia; Rothlein, Robert; Sellati, Rosemarie H.; Woska, Joseph R., Jr.; Chen, Shirlynn; Gunn, Jocelyn A.; O'Brien, Drane; Norris, Stephen H.; ***Kelly, Terence A.***; Peng, Charline; ***Wu, Jiang-Ping***

CORPORATE SOURCE: Research and Development, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(22), 5356-5366
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:6469

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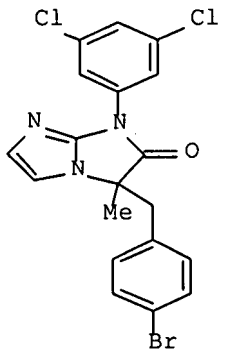

I

AB A novel class of lymphocyte function-associated antigen-1 (LFA-1) inhibitors is described. Discovered during the process to improve the physicochem. and metabolic properties of BIRT377, a previously reported hydantoin-based LFA-1 inhibitor, these compds. are 5- or 6-substituted derivs. of the 1H-imidazo[1,2-α]imidazol-2-one I. The structure-activity relationship (SAR) shows that electron-withdrawing groups at C(5) on the imidazole ring benefit potency and that oxygen-containing functional groups attached to a C(5)-sulfonyl or sulfonamide group further improve potency. This latter gain in potency is attributed to the interaction(s) of the functionalized sulfonyl/sulfonamide groups with the protein, likely polar-polar in nature, as suggested by SAR data. X-ray studies revealed that these bicyclic inhibitors bind to the I-domain of LFA-1 in a pattern similar to that of BIRT377.

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT ***321656-72-8P 321719-80-6P 321721-16-8P 321721-24-8P 321722-24-1P 321723-65-3P 321723-77-7P***
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-imidazo[1,2-α]imidazol-2-ones as second-generation

lymphocyte function-associated antigen-1 inhibitors)

IT *321656-35-3P 321656-61-5P 321656-73-9P*
321656-95-5P 321657-00-5P 321657-01-6P
321657-02-7P 321657-04-9P 321718-99-4P
321720-06-3P 321720-66-5P 321720-72-3P
321720-89-2P 321721-28-2P 321722-68-3P
321722-90-1P 321722-94-5P 321723-35-7P
321723-54-0P 321723-68-6P 321723-69-7P
321723-71-1P 321723-75-5P 796871-98-2P
796871-99-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 1H-imidazo[1,2-α]imidazol-2-ones as second-generation lymphocyte function-associated antigen-1 inhibitors)

IT 213209-22-4P *321656-74-0P 321656-99-9P* 321724-07-6P
321724-14-5P 321724-15-6P 321724-16-7P 321724-18-9P,
2-Azidomethyl-1,3-dioxolane *796872-00-9P 796872-01-0P*
796872-02-1P 796872-03-2P 796872-04-3P 797762-16-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-imidazo[1,2-α]imidazol-2-ones as second-generation lymphocyte function-associated antigen-1 inhibitors)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:412950 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:423947
TITLE: Preparation of [6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonylamino]propionamide derivatives for treatment of inflammatory disease
INVENTOR(S): ***Kelly, Terence Alfred***; Kim, Jin Mi; ***Lemieux, Rene Marc***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041827	A2	20040521	WO 2003-US333865	20031027
WO 2004041827	A3	20040715		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004127534	A1	20040701	US 2003-686073	20031015
US 6844360	B2	20050118		
CA 2504219	A1	20040521	CA 2003-2504219	20031027
AU 2003284938	A1	20040607	AU 2003-284938	20031027
EP 1560830	A2	20050810	EP 2003-779257	20031027

EP 1560830		B1	20061025			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK						
BR 2003015836		A	20050913	BR 2003-15836		20031027
CN 1708500		A	20051214	CN 2003-80102491		20031027
JP 2006508947		T	20060316	JP 2004-550109		20031027
EP 1712553		A2	20061018	EP 2006-118540		20031027
EP 1712553		A3	20061102			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK						
AT 343582		T	20061115	AT 2003-779257		20031027
NZ 540269		A	20070531	NZ 2003-540269		20031027
US 2005054703		A1	20050310	US 2004-969105		20041020
US 2005165027		A1	20050728	US 2005-34701		20050113
ZA 2005002701		A	20051013	ZA 2005-2701		20050404
NO 2005002579		A	20050527	NO 2005-2579		20050527
PRIORITY APPLN. INFO.:				US 2002-422446P	P	20021030
				US 2003-686073	A3	20031015
				EP 2003-779257	A3	20031027
				WO 2003-US33865	W	20031027

OTHER SOURCE(S): MARPAT 140:423947

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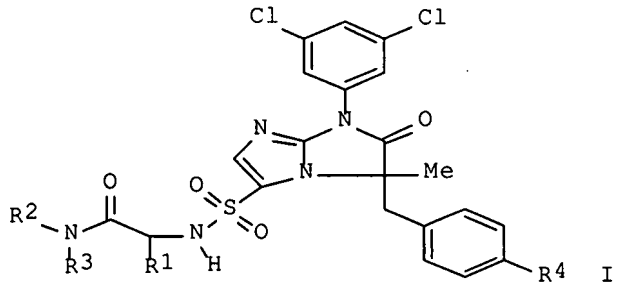

I

AB The invention relates to imidazo[1,2-a]imidazole amino acid derivs. I [R1 is alkyl optionally mono- or disubstituted by oxo or morpholino; R2, R3 are H or alkyl mono- or disubstituted by CONH2 or OH or R2R3N is piperazinyl; R4 is cyano, trifluoromethoxy, pyrimidinyl or mono- or diaminopyrimidinyl] or their pharmaceutically-acceptable salts which exhibit good inhibitory effect upon the interaction of cellular adhesion mols. (CAMs) and leukointegrins and are thus useful in the treatment of inflammatory disease. Thus, I [R2R3NCOCHR1NH is L-alaninamide residue (R ring stereo)] was prepared from (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)- 3-methyl-1H-imidazo[1,2-a]imidazol-2-one by cyanation with Zn(CN)2, conversion to the sulfonyl chloride (iodination with N-iodosuccinimide, reaction with cyclopentylmagnesium chloride, SO2 and N-chlorosuccinimide), and condensation with L-alaninamide hydrochloride. Synthesized I showed Kd < 10 μM for inhibition of integrin LFA-1 and ICAM-1.

IC ICM C07D487-04
ICS A61K031-4164; A61P037-00; C07D235-00

CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 28, 63

IT ***688755-94-4P 688755-95-5P 688755-96-6P 688755-97-7P 688755-98-8P 688755-99-9P***

688756-00-5P 688756-01-6P 688756-02-7P
688756-03-8P 688756-04-9P 688756-05-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [(dihydroimidazoimidazolesulfonyl)amino]propionamide derivs.
for treatment of inflammatory disease)

IT 1072-97-5, 5 Bromo 2 pyridinamine 1668-10-6, Glycinamide hydrochloride 6160-65-2, Thiocarbonyldiimidazole 13404-22-3, L-Alanine tert butyl ester hydrochloride 22483-09-6, Aminoacetaldehyde dimethyl acetal 32916-51-1, Cyclopentylmagnesium chloride 33208-99-0, L-Alaninamide hydrochloride 50824-05-0, 4 Trifluoromethoxybenzyl bromide 71810-97-4, D-Alaninamide hydrochloride 73183-34-3 ***321656-72-8*** 321724-17-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of [(dihydroimidazoimidazolesulfonyl)amino]propionamide derivs.
for treatment of inflammatory disease)

IT 110-91-8P, Morpholine, preparation 30924-93-7P 86150-09-6P 124212-41-5P ***321657-06-1P 321657-07-2P 688756-06-1P 688756-07-2P 688756-08-3P 688756-09-4P 688756-10-7P*** 688756-11-8P 688756-12-9P 688756-13-0P 688756-14-1P 688756-15-2P 688756-16-3P ***688756-17-4P 688756-18-5P 688756-19-6P*** 689261-01-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of [(dihydroimidazoimidazolesulfonyl)amino]propionamide derivs.
for treatment of inflammatory disease)

L23 ANSWER 9 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:412808 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:423673
TITLE: Preparation of derivatives of [6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl]-pyrrolidine-2-carboxylic acid amide as anti-inflammatory agents
INVENTOR(S): ***Kelly, Terence Alfred***; Kim, Jin Mi; ***Lemieux, Rene Marc***; Tschantz, Matt Aaron
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041273	A1	20040521	WO 2003-US333966	20031027

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 6852748	B1	20050208	US 2003-685638	20031015
CA 2504131	A1	20040521	CA 2003-2504131	20031027
AU 2003286700	A1	20040607	AU 2003-286700	20031027
EP 1558248	A1	20050803	EP 2003-777910	20031027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508106	T	20060309	JP 2004-550125	20031027
US 2005054704	A1	20050310	US 2004-969698	20041020
PRIORITY APPLN. INFO.:			US 2002-422449P	P 20021030
			US 2003-685638	A3 20031015
			WO 2003-US33966	W 20031027

OTHER SOURCE(S): MARPAT 140:423673

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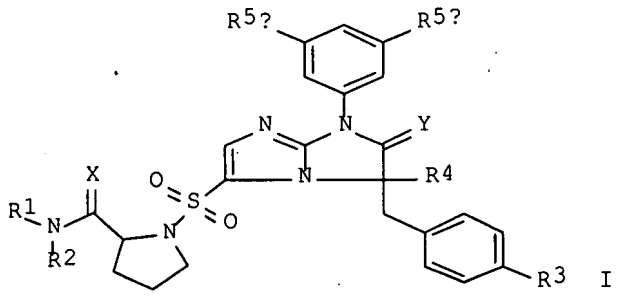


I

AB The title compds. [I; R1, R2 = hydrogen (provided that R1 and R2 are not both hydrogen atoms), each (un)substituted straight or branched C1-7 alkyl, C3-6 cycloalkyl, aryl (selected form the group consisting of biphenyl, Ph, or quinolinyl), or unsatd. or partially saturated heterocyclic group containing 2 to 3 C, 1 to 2 N, 0 to 1 S, and 0 to 1 O atoms; or wherein R1 and R2 constitute a saturated 3 to 5-methylene group bridge which together with the nitrogen atom between them form (un)substituted heterocyclic ring; R3 = (un)substituted aryl (selected from the group consisting of pyridyl and pyrimidyl), CF3O, cyano; R4 = straight or branched C1-3 alkyl; R5a, R5b = Cl, CF3; X, Y = O, S; Y] or pharmaceutically acceptable salts thereof are prepared These compds. exhibit good inhibitory effect upon the interaction of cellular adhesion mols. (CAMs) and leukointegrins and are thus useful in the treatment of inflammatory disease including adult respiratory distress syndrome, shock, oxygen toxicity, multiple organ injury syndrome secondary to septicemia, multiple organ injury syndrome secondary to trauma, reperfusion injury of tissue due to cardiopulmonary bypass, myocardial infarction [associated with use of thrombolysis agents (sic)], acute glomerulonephritis, vasculitis, reactive arthritis, dermatosis with acute inflammatory components, stroke, thermal injury, hemodialysis, leukapheresis, ulcerative colitis, necrotizing enterocolitis, granulocyte transfusion associated syndrome, psoriasis, organ/tissue transplant rejection, graft vs. host reactions, autoimmune diseases (including Raynaud's syndrome, autoimmune thyroiditis, dermatitis, multiple sclerosis, rheumatoid arthritis, insulin-dependent diabetes mellitus, uveitis, inflammatory bowel disease, Crohn's disease, ulcerative colitis or systemic lupus erythematosus), asthma, or the toxic effects of cytokine therapy. Thus, a solution of (R)-3-(3,5-dichlorophenyl)- 5-methyl-2-thioxo-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one and aminoacetaldehyde dimethylacetal (6.50 mL, 59.7 mmol) in MeOH was treated with aqueous tert-Bu hydroperoxide solution over 25 min at <20° under ice-cooling, kept at the same

temperature for 1 h , warmed to room temperature, and stirred for 86 h to give (R)-3-(3,5-dichlorophenyl)-2-[((E)-2,2- dimethoxyethyl)imino]-5-methyl-5-(4-trifluoromethoxybenzyl)imidazolidin-4- one which was heated in the presence of p-MeC6H4SO3H in acetone at reflux for 2 h to give (R)-1-(3,5-dichlorophenyl)-3-methyl-3-(4- trifluoromethoxybenzyl)-1H-imidazo[1,2-a]imidazol-2-one.

IC ICM A61K031-4188
ICS C07D487-04; A61P029-00

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 2854-16-2P, 2-Hydroxy-2-methylpropyl-1-amine 86150-21-2P, (S)-Pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide 102774-95-8P, (R)-(-)-Dihydro-5-(azidomethyl)-2(3H)-furanone 137862-22-7P, (S)-1-(tert-Butoxycarbonyl)pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide ***321656-41-1P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ***321656-51-3P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid amide ***321657-06-1P***, (R)-3-(4-Cyanobenzyl)-1-(3,5-dichlorophenyl)-3-methylimidazo[1,2-a]imidazol-2-one ***321657-07-2P***, (R)-5-(4-Bromobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride ***321724-08-7P***, (R)-3-(4-Cyanobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one ***688756-08-3P***, (R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride 688756-14-1P, (2R,5R)-2-tert-Butyl-3-(3,5-dichlorophenyl)-5-methyl-1-(2,2,2-trifluoroacetyl)-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one 688756-15-2P, (R)-2-Amino-N-(3,5-dichlorophenyl)-2-methyl-3-(4-trifluoromethoxyphenyl)propionamide 688756-16-3P, (R)-3-(3,5-Dichlorophenyl)-5-methyl-2-thioxo-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one ***688756-18-5P***, (R)-1-(3,5-Dichlorophenyl)-5-iodo-3-methyl-3-(4-trifluoromethoxybenzyl)-1H-imidazo[1,2-a]imidazol-2-one 689261-01-6P, (R)-3-(3,5-Dichlorophenyl)-2-[((E)-2,2-dimethoxyethyl)imino]-5-methyl-5-(4-trifluoromethoxybenzyl)imidazolidin-4-one ***691906-14-6P*** ***691906-17-9P***, 1-[[(S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]piperidine-4-carboxylic acid methyl ester 691906-26-0P, (S)-Pyrrolidine-2-carboxylic acid N-(2-hydroxy-2-methylpropyl)amide hydrochloride ***691906-29-3P*** ***691906-30-6P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid tert-butyl ester ***691906-90-8P***, (S)-2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-3-(tert-butoxy)propionic acid tert-butyl ester ***691906-93-1P***, (S)-1-[[(R)-5-(4-Bromobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide ***691906-94-2P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of [dihydro-5H-imidazo[1,2-a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)

IT ***321656-42-2P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of [dihydro-5H-imidazo[1,2-a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)

IT ***688756-17-4P***, (R)-1-(3,5-Dichlorophenyl)-3-methyl-3-(4-trifluoromethoxybenzyl)-1H-imidazo[1,2-a]imidazol-2-one ***691906-09-9P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-hydroxy-2-methylpropyl)amide ***691906-11-3P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-hydroxyethyl)amide ***691906-12-4P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(carbamoylmethyl)amide ***691906-13-5P***, (R)-2-[[[(S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid ***691906-15-7P***, [[[(S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]acetic acid ***691906-16-8P***, 1-[[(S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]piperidine-4-carboxylic acid ***691906-18-0P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-((S)-2-hydroxypropyl)amide ***691906-19-1P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-1,1-dimethylethyl)amide ***691906-20-4P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(furan-2-ylmethyl)amide ***691906-21-5P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4-hydroxyphenyl)amide ***691906-22-6P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(3-hydroxyphenyl)amide ***691906-23-7P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid acetylamide ***691906-24-8P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-[((R)-5-oxotetrahydrofuran-2-yl)methyl]amide ***691906-25-9P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide ***691906-27-1P*** ***691906-28-2P***, (S)-1-[[(R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide ***691906-31-7P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-methoxyethyl)amide ***691906-32-8P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-acetylaminoethyl)amide ***691906-33-9P*** ***691906-34-0P*** ***691906-35-1P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-

imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide ***691906-36-2P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide ***691906-37-3P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid [2-(morpholin-4-yl)ethyl]amide ***691906-38-4P*** ***691906-39-5P***, [2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]ethyl]carbamic acid tert-butyl ester ***691906-40-8P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-aminoethyl)amide ***691906-41-9P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (3-hydroxypropyl)amide ***691906-42-0P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(furan-2-ylmethyl)amide ***691906-43-1P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2,3-dihydroxypropyl)amide ***691906-44-2P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-1-methylethyl)amide ***691906-45-3P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(cyanomethyl)amide ***691906-46-4P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-((R)-2-hydroxy-1-methylethyl)amide ***691906-47-5P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-((S)-1-hydroxymethyl-3-methylbutyl)amide ***691906-48-6P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((R)-1-hydroxymethyl-3-methylbutyl)amide ***691906-49-7P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid [2-hydroxy-1-(hydroxymethyl)ethyl]amide ***691906-50-0P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-aminophenyl)amide ***691906-51-1P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(3-aminophenyl)amide ***691906-52-2P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4-aminophenyl)amide ***691906-53-3P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(biphenyl-4-yl)amide ***691906-54-4P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(quinolin-6-yl)amide ***691906-55-5P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid

N-[4-(morpholin-4-yl)phenyl]amide ***691906-56-6P***,
(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(1-methyl-4-oxo-4,5-dihydro-1H-imidazol-2-yl)amide ***691906-57-7P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(1,3,5-trimethyl-1H-pyrazol-4-yl)amide ***691906-58-8P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4-oxo-4,5-dihydrothiazol-2-yl)amide ***691906-59-9P***
691906-60-2P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(2-ethyl-2H-pyrazol-3-yl)amide ***691906-61-3P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-1,1-dimethylethyl)amide ***691906-62-4P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((S)-2-hydroxypropyl)amide ***691906-63-5P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((R)-2-hydroxypropyl)amide ***691906-64-6P***, (R)-1-(3,5-Dichlorophenyl)-5-[[(S)-2-[(R)-3-hydroxypyrrolidin-1-yl)carbonyl]pyrrolidin-1-yl]sulfonyl]-3-methyl-3-[4-(pyrimidin-5-yl)benzyl]-1H-imidazo[1,2-a]imidazol-2-one ***691906-65-7P***,
(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-methyl-N-(carbamoylmethyl)amide ***691906-66-8P***
, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((S)-1-methylcarbamoylethyl)amide ***691906-67-9P***
, 1-[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]piperidine-4-carboxylic acid amide ***691906-68-0P***,
(R)-1-(3,5-Dichlorophenyl)-5-[[(S)-2-[(S)-3-hydroxypyrrolidin-1-yl)carbonyl]pyrrolidin-1-yl]sulfonyl]-3-methyl-3-[4-(pyrimidin-5-yl)benzyl]-1H-imidazo[1,2-a]imidazol-2-one ***691906-69-1P***,
1-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]cyclopropanecarboxylic acid methyl ester
691906-70-4P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(4,5-dihydrooxazol-2-yl)amide
691906-71-5P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(1H-tetrazol-5-ylmethyl)amide
691906-72-6P, (R)-2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid
691906-73-7P, (S)-2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid
691906-74-8P, [[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]acetic acid
691906-75-9P, [N-[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]-N-methylamino]acetic acid

691906-76-0P, 2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-2-methylpropionic acid
691906-77-1P, 3-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]propionic acid
691906-78-2P, 1-[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]piperidine-4-carboxylic acid
691906-79-3P, 6,7-Dihydro-3-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-4,4,4-trifluorobutyric acid methyl ester ***691906-80-6P***, 3-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-4,4,4-trifluorobutyric acid ethyl ester
691906-81-7P, (S)-2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl](methyl)amino]-3-methylbutyric acid
691906-82-8P, (1S,2S)-2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]cyclohexanecarboxylic acid ***691906-83-9P***, 3-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]butyric acid
691906-84-0P, 3-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-2-methylpropionic acid
691906-85-1P, 1-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]cyclopropanecarboxylic acid
691906-86-2P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-carbamoylethyl)amide
691906-87-3P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid ((R)-1-carbamoylethyl)amide
691906-88-4P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (1-carbamoyl-1-methylethyl)amide
691906-89-5P, (S)-2-[[[(S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-[4-(pyrimidin-5-yl)benzyl]-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidin-2-yl]carbonyl]amino]-3-hydroxypropionic acid
691906-91-9P, (S)-1-[[(R)-5-[4-(4-Aminopyrimidin-5-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide ***691906-95-3P***, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-[4-(2-fluoropyrimidin-5-yl)benzyl]-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide ***691906-96-4P***, (S)-1-[[(R)-5-[4-(4-Aminopyrimidin-5-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide
691906-97-5P, (S)-1-[[(R)-7-(3,5-Dichlorophenyl)-5-[4-(2-fluoropyrimidin-5-yl)benzyl]-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxyethyl)amide ***691906-98-6P***, (S)-1-[[(R)-5-[4-(2-Cyanopyridin-3-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide ***691906-99-7P***,

(S)-1-[[(R)-5-[4-(2-Cyanopyridin-3-yl)benzyl]-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl]sulfonyl]pyrrolidine-2-carboxylic acid N-(carbamoylmethyl)amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [dihydro-5H-imidazo[1,2-a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)

IT ***688756-19-6P***, (R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of [dihydro-5H-imidazo[1,2-a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)

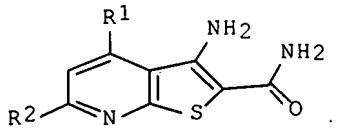
IT 75-86-5, Acetone cyanohydrin 98-74-8, 4-Nitrobenzenesulfonyl chloride 108-24-7, Acetic anhydride 109-85-3, 2-Methoxyethylamine 141-43-5, Ethanolamine, reactions 1668-10-6, Glycinamide hydrochloride 2799-17-9, (S)-1-Aminopropan-2-ol 2812-46-6 2971-79-1, Methyl isonipecotate 3196-73-4, β-Alanine methyl ester hydrochloride 15761-39-4 22483-09-6, Aminoacetaldehyde dimethylacetal 32916-51-1, Cyclopentylmagnesium chloride 33240-34-5, Cyclopentylmagnesium bromide 42429-27-6 48067-24-9, O-tert-Butyl-L-serine tert-butyl ester 50824-05-0, 4-Trifluoromethoxybenzyl bromide 52813-63-5, (R)-(-)-Dihydro-5-(hydroxymethyl)-2(3H)-furanone 53742-62-4, N-(tert-Butyldimethylsilyl)aniline 59531-86-1, D-Alanine tert-butyl ester hydrochloride 59624-87-2 73183-34-3 ***321656-72-8***, (R)-3-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-3-methylimidazo[1,2-a]imidazol-2-one ***321656-73-9***, (R)-3-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one 321724-17-8, (2S,5R)-2-tert-Butyl-3-(3,5-dichlorophenyl)-5-methyl-1-(2,2,2-trifluoroacetyl)imidazolidin-4-one 321724-19-0, 5-(4,4,5,5-Tetramethyl-[1,3,2]dioxaborolan-2-yl)pyrimidine 343926-69-2, 2-Amino-4-bromopyrimidine 691906-10-2, (S)-2-(2-Hydroxy-2-methylpropylcarbamoyl)pyrrolidine-1-carboxylic acid tert-butyl ester 691906-92-0, L-Pyrrolidine-2-carboxylic acid (2-hydroxy-2-methylpropyl)amide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of [dihydro-5H-imidazo[1,2-a]imidazolylsulfonyl]pyrrolidinecarboxylic acid amide derivs. for treatment of inflammatory diseases)

L23 ANSWER 10 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:991342 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:42161
TITLE: Preparation of substituted 3-amino-thieno[2,3-b]pyridine-2-carboxylic acid amide compounds and processes for preparing and their uses as inhibitors of IκB kinase complex
INVENTOR(S): Cywin, Charles L.; Chen, Zhidong; ***Emeigh, Jonathan***; Fleck, Roman Wolfgang; Hao, Ming-hong; Hickey, Eugene; Liu, Weimin; Marshall, Daniel Richard; Morwick, Tina; Nemoto, Peter; ***Sorcek, Ronald John***; Sun, Sanxing; ***Wu, Jiang-ping***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 165 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003103661	A1	20031218	WO 2003-US17343		20030603
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2483890	A1	20031218	CA 2003-2483890		20030603
AU 2003237330	A1	20031222	AU 2003-237330		20030603
US 2004053957	A1	20040318	US 2003-453175		20030603
US 6964956	B2	20051115			
BR 2003011605	A	20050222	BR 2003-11605		20030603
EP 1513516	A1	20050316	EP 2003-736796		20030603
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1649581	A	20050803	CN 2003-809958		20030603
JP 2005530816	T	20051013	JP 2004-510780		20030603
NZ 537394	A	20061222	NZ 2003-537394		20030603
US 2004180922	A1	20040916	US 2003-730172		20031206
US 6974870	B2	20051213			
IN 2004DN03224	A	20050401	IN 2004-DN3224		20041019
NO 2004004599	A	20050216	NO 2004-4599		20041025
US 2005288285	A1	20051229	US 2005-206707		20050818
PRIORITY APPLN. INFO.:			US 2002-386312P	P	20020606
			US 2003-457867P	P	20030326
			US 2003-453175	A1	20030603
			WO 2003-US17343	W	20030603

OTHER SOURCE(S): MARPAT 140:42161
GI



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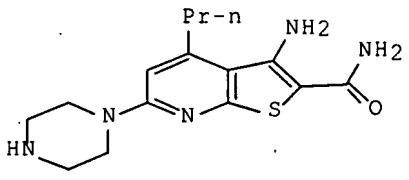

II

AB Title compds. I [R1 = (un)substituted-Ph, -heteroaryl, -heterocyclyl, -alkyl, -alkoxy, etc.; R2 = (un)substituted-alkyl, -alkoxy, -alkylamino, -alkylthio, -Ph, -heterocyclyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of the kinase activity of the IκB kinase (IKK) complex. Thus, e.g., II was prepared in five steps by cyclization of Me 2-hexynoate with 2-cyanothioacetamide in the presence of morpholine to provide intermediate mercaptopyridone which is S-alkylated with 2-bromoacetamide,

converted to the O-triflate derivative, reacted with 1-BOC-piperazine and deprotected. I possessed IC50's of 10 μM or below in assays for inhibition of IKKβ. The compds. are therefore useful in the treatment of IKK mediated diseases including autoimmune diseases, inflammatory diseases and cancer. Also disclosed are pharmaceutical compns. comprising these compds. and processes for preparing these compds.

IC ICM A61K031-38
ICS A61K031-435; C07D495-04; A61P029-00; C07D333-00; C07D221-00
CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 11 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:487567 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:52411
TITLE: Small molecules useful in the treatment of inflammatory disease
INVENTOR(S): Fleck, Roman Wolfgang; ***Kelly, Terence Alfred***; Kim, Jin Mi; Lee, Jinbo; ***Lemieux, Rene Marc***; ***Sorcek, Ronald John***; ***Wu, Jiang-Ping***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002050080	A1	20020627	WO 2001-US46649	20011205
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 2003008848	A1	20030109	US 2001-11070	20011205
PRIORITY APPLN. INFO.:			US 2000-256811P P	20001219

OTHER SOURCE(S): MARPAT 137:52411
AB A method for treating or preventing inflammatory and immune cell-mediated diseases by the administration of certain small heterocyclic compds. are described. These compds. act by inhibiting interaction of cellular adhesion mols. (including ICAM-1, ICAM-2, and ICAM-3) with the leukointegrins (especially CD18/CD11a). Pharmaceutical compns. comprising these small heterocyclic compds., such as capsules, tablets, parenteral solns., suspensions or topical formulations, suitable for the prevention or treatment of inflammatory and immune cell-mediated diseases are also described.
IC ICM C07D487-04
ICS C07D498-04; C07D495-04; C07D513-04; C07D491-04; A61K031-41
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1, 28
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 12 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:182177 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:232302
TITLE: Preparation of 1-phenyl-2,5-imidazolidinediones and analogs for treatment of inflammatory and immune cell-mediated diseases

INVENTOR(S): ***Kelly, Terence A.***; Bormann, Barbara Jean; Frye, Leah Lynn; ***Wu, Jiang-Ping***

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: U.S., 114 pp., Cont.-in-part of Appl. No. PCT/US98/04254.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6355664	B1	20020312	US 1999-375010	19990816
WO 9839303	A1	19980911	WO 1998-US4254	19980303
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 38132	E1	20030603	US 2002-167732	20020612

PRIORITY APPLN. INFO.:

US 1997-40011P	P	19970303
US 1998-33148	B2	19980302
WO 1998-US4254	A2	19980303
US 1999-375010	A5	19990816

OTHER SOURCE(S): MARPAT 136:232302

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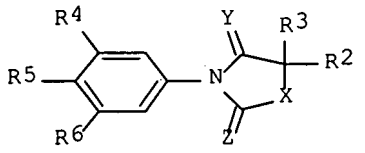

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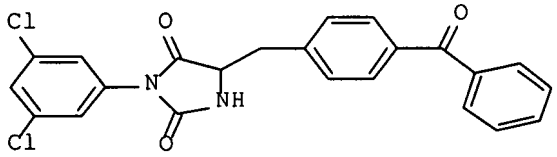

II

AB Title imidazolidinediones, pyrrolidinediones, oxazolidinediones, and thiazolidinediones I [wherein Y = O or S; Z = O or S; X = CHR1, NR1, CHSO2R1, or NSO2R1; R1 = H, carboxylic acid group, phosphonic acid group, sulfonic acid group, imidamidoalkyl, guanidinoalkyl, or (un)substituted (cyclo)alkyl, piperidyl, or aryl; R2 = H or (un)substituted (cyclo)alkyl; R3 = H or (un)substituted aryl(alkyl); R4 = Cl or CF3; R5 and R6 = independently H, halo, Me, or CF3; and pharmaceutically acceptable salts] were prepared as intracellular adhesion mols. (ICAMs) and leukointegrin antagonists. For example, reaction of 4-benzoyl-DL-phenylalanine with 3,5-

dichlorophenylisocyanate and cyclization of the ureidoacetic acid intermediate gave II. The latter inhibited lymphocyte function-associated 1 (LFA-1) binding to ICAM-1 with Kd of 1.64 μM. I are useful for the treatment of inflammatory and immune cell-mediated disorders, such as psoriasis, organ/tissue transplant rejection, graft vs. host reactions, autoimmune diseases, asthma, and toxicity associated with cytokine therapy.

IC ICM A61K031-4439
ICS A61K031-4166; C07D401-10; C07D233-40
INCL 514389000
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 34
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 13 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:202160 ZCAPLUS Full-text
TITLE: Small molecule antagonists of LFA-1 mediated cell adhesion
AUTHOR(S): ***Emeigh, Jonathan E.***; Bormann, Barbara-Jean; Frye, Leah L.; Jeanfavre, Deborah D.; McNeil, Daniel W.; Nabozny, Gerald H.; Stefany, David W.; Woska, Joseph R., Jr.; ***Wu, Jiang-Ping***; Zindell, Renee; Zinter, Rosemary; ***Kelly, Terence A.***
CORPORATE SOURCE: Medicinal Chemistry Department, Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT, 06810, USA
SOURCE: Abstracts of Papers, 221st ACS National Meeting, San Diego, CA, United States, April 1-5, 2001 (2001)
MEDI-256
CODEN: 69FZD4
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; Meeting Abstract
LANGUAGE: English
AB Lymphocyte function-associated antigen 1 (LFA-1) is a cellular adhesion mol. involved in many fundamental immunol. processes such as leukocyte trafficking, antigen presentation, B-cell activation, and activation of cytotoxic T lymphocytes. Modulation of these LFA-1 mediated events may lead to useful therapeutic agents for autoimmune disorders. In this poster, we report on the structure-activity relationships of a novel class of small mols. (e.g. BIRT0377) that blocks the interactions between LFA-1 and one of its adhesion partners, ICAM-1.

L23 ANSWER 14 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:78387 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:131538
TITLE: Preparation of imidazoimidazoles and triazoles as anti-inflammatory agents
INVENTOR(S): ***Wu, Jiang-Ping; Kelly, Terence Alfred; Lemieux, Rene M.; Goldberg, Daniel R.; Emeigh, Jonathan Emilian; Sorcek, Ronald J.***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 368 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2001007440	A1	20010201	WO 2000-US18884	20000712
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6492408	B1	20021210	US 2000-604312	20000627
CA 2383017	A1	20010201	CA 2000-2383017	20000712
BR 2000012666	A	20020409	BR 2000-12666	20000712
EP 1216247	A1	20020626	EP 2000-948618	20000712
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200160	T2	20021021	TR 2002-160	20000712
JP 2003505460	T	20030212	JP 2001-512524	20000712
HU 200203971	A2	20030328	HU 2002-3971	20000712
EE 200200028	A	20030415	EE 2002-28	20000712
NZ 517217	A	20040227	NZ 2000-517217	20000712
AU 776496	B2	20040909	AU 2000-62091	20000712
TW 261591	B	20060911	TW 2000-89114536	20000720
IN 2002MN00002	A	20060915	IN 2002-MN2	20020102
BG 106312	A	20020930	BG 2002-106312	20020116
ZA 2002000428	A	20030117	ZA 2002-428	20020117
NO 2002000275	A	20020204	NO 2002-275	20020118
NO 322707	B1	20061127		
US 2003203955	A1	20031030	US 2002-195973	20020716
US 6689804	B2	20040210		
HK 1048637	A1	20050225	HK 2003-100839	20030206
US 2004116426	A1	20040617	US 2003-672412	20030925
PRIORITY APPLN. INFO.:			US 1999-144905P	P 19990721
			US 1999-150939P	P 19990826
			US 2000-604312	A1 20000627
			WO 2000-US18884	W 20000712
			US 2002-195973	A3 20020716
OTHER SOURCE(S):	MARPAT 134:131538			

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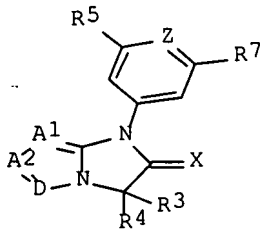

I

AB Compds. I {A1 = N, CH; A2 = N, CH, CR'; R' = halo, cyano, alkoxy, alkoxycarbonyl, alkylsulfonyl; D = N, CH, CR1, C(SO2R1), C[S(:O)R1], C(CHO),

C(SR1a), C(OR1a), C(NHR1a); R1, R1a = (substituted) alkyl, cycloalkyl, aryl, or heteroaryl groups, alkyl groups containing 2-6 carbons substituted with carboxylate, phosphonate, sulfonate, amidine, or guanidine moieties, amino, halogen, cyano; R3 = H, alkyl, cycloalkyl, alkoxy or amino substituted alkyl, cycloalkyl; R4 = substituted arylmethyl; R5 = Cl, F3C; R7 = H, halo, Me, cyano, O2N, F3C; X = O, S; if Z = N or CH, R7 = Cl, F3C, cyano, O2N; Z = N, CR6 where R6 = H, halo, Me, cyano, F3C}, based mostly on imidazo[1,2-a]imidazole and imidazo[1,2-a]triazole nuclei, are prepared as inhibitors of the binding of leukointegrins to cell adhesion mols. in the treatment or prevention of inflammatory and immune cell-mediated diseases. E.g., (R)-I (A1 = N; A2 = D = CH; R3 = Me; R4 = 4-BrC6H4CH2; R5 = R7 = Cl; X = O; Z = CH) (II) was prepared from (R)-α-methyl-4-bromophenylalanine Me ester and 3,5-dichlorophenylisothiocyanate by heating in 1,4-dioxane to give a thiohydrantoin which was treated with N-(triphenylphosphoranylidene)-1,3-dioxolan-2-ylmethylamine [prepared from 2-(azidomethyl)-1,3-dioxolane and triphenylphosphine] to give a dioxolanylmethyliminoimidazolidinone derivative; treatment of the intermediate with trifluoroacetic acid and heating at 90° overnight gave II with m.p. 36-37.5°. I inhibited binding of leukointegrins to cell adhesion mols. with Kd<10 μM.

IC ICM C07D487-04
ICS C07F009-40; C07D519-00; C07F009-38; A61K031-41; A61K031-415; A61P029-00; C07D487-04; C07D233-00; C07D487-04; C07D233-00; C07D249-00; C07D487-04; C07D233-00; C07D257-00

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT *321656-35-3P 321656-59-1P 321656-61-5P*
321656-64-8P 321656-68-2P 321656-72-8P
321656-73-9P 321656-74-0P 321656-99-9P
321657-06-1P 321657-07-2P 321657-64-1P
321724-09-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

IT *321656-36-4P 321656-37-5P 321656-38-6P*
321656-39-7P 321656-41-1P 321656-42-2P
321656-43-3P 321656-51-3P 321656-52-4P
321656-53-5P 321656-54-6P 321656-57-9P
321656-58-0P 321656-60-4P 321656-62-6P
321656-63-7P 321656-65-9P 321656-66-0P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of

inflammatory and immune-cell mediated diseases)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

IT *321724-20-3P*
RL: BYP (Byproduct); PREP (Preparation)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

IT 110-85-0, Piperazine, reactions 874-24-8, 3-Hydroxypicolinic acid 1692-25-7, 3-Pyridineboronic acid 2133-40-6, L-Proline methyl ester hydrochloride 3235-69-6, 4-Morpholineacetic acid 6165-69-1, 3-Thiopheneboronic acid 13889-98-0, N-Acetylpiperazine 17201-43-3, α-Bromo-p-tolunitrile 50585-89-2, Methyl nipecotate 57260-71-6 69849-42-9, 5-(Trimethylstannyl)pyrimidine 131534-65-1 156545-07-2, 3,5-Difluorophenylboronic acid *321724-14-5 321724-15-6* 321724-16-7 321724-17-8 321724-18-9 321724-19-0 321724-21-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of

inflammatory and immune-cell mediated diseases)

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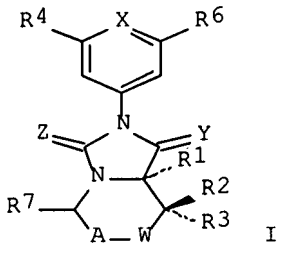
321724-13-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazoimidazole and imidazotriazole derivs. as inhibitors of leukointegrin binding to cell adhesion mols. in the treatment of inflammatory and immune-cell mediated diseases)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 15 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:78243 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:131537
TITLE: Novel N-aryl cycloalkyl fused imidazolediones useful in the treatment of inflammatory disease
INVENTOR(S): ***Kelly, Terence Alfred; Wu, Jiang-Ping***; Kuzmich, Daniel
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007052	A1	20010201	WO 2000-US17752	20000628
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6365615	B1	20020402	US 2000-605675	20000628
PRIORITY APPLN. INFO.:			US 1999-144894P	P 19990721

OTHER SOURCE(S): MARPAT 134:131537
GI



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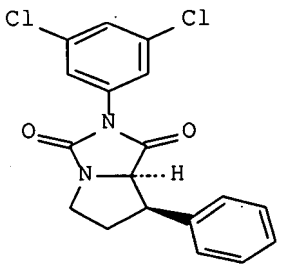

II

AB Novel N-aryl cycloalkyl fused imidazolediones I [Y and Z independently = O or S; R1 = H, (un)substituted unbranched or branched alkyl or cycloalkyl, alkoxy or acyloxy; R2 = (un)substituted aryl; R3 = H, OH, alkoxy, acyloxy, or (un)substituted unbranched or branched alkyl or cycloalkyl; R4 = Cl or CF3; X

= N or CR5 where R5 = H, halo, Me, or CF3; R6 = H, halo, Me, CN, NO2 or CF3 with condition that when X = N or CH, R6 = Cl or CF3; A = (CHR8)m where m = 0 or 1; W = (CHR9)n where n = 0 or 1 and m + n = 1 or 2; R7, R8 and R9 independently = H, oxo, R10, OR10, NHR10, COR10, CONHR10, CO2R10, SO2R10 or SR10 wherein R10 = H, (un)substituted branched or unbranched alkyl or cycloalkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamidino, etc.] which are useful for treating or preventing inflammatory and immune cell-mediated diseases are disclosed as well as methods for their preparation Thus, II was prepared in four steps via a cyclocondensation reaction of an intermediate N-(3,5-dichlorophenylamido)- 3-phenylpyrrolidin-2-yl carboxylic acid. The title compds. possessed Kd values < 10 μM for inhibition of LFA-1 binding to ICAM-1. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K031-55
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 16 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:78239 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:131536
TITLE: Novel N-(pyridin-4-yl) nitrogen heterocyclic compounds useful in the treatment of inflammatory disease
INVENTOR(S): ***Kelly, Terence Alfred; Sorcek, Ronald John***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007048	A1	20010201	WO 2000-US17806	20000628
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6350763	B1	20020226	US 2000-604899	20000628
PRIORITY APPLN. INFO.:			US 1999-144844P P	19990721

OTHER SOURCE(S): MARPAT 134:131536
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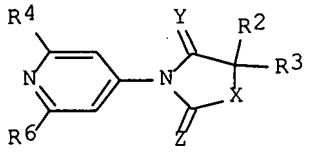

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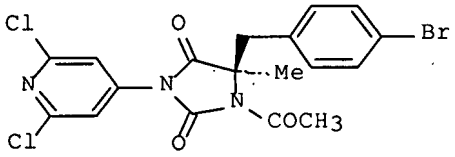

II

AB Novel N-(pyridin-4-yl) nitrogen heterocyclic compds. I [Y and Z are independently O or S; X = O, S, CHR1, NR1, CHSO2R1 or NSO2R1; R1 = H, (un)substituted branched or unbranched alkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamidino, N-substituted piperidyl, etc.; R2 = H, (un)substituted branched or unbranched alkyl or cycloalkyl; R3 = (CR7R8)x(CR9R10)yR11 where x and y independently = 0 or 1; R7, R8, and R9 independently = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl; R10 = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl, (un)substituted aryl; R11 = (un)substituted aryl; R4 = Cl, CF3; R6 = halo, Me, CF3, CN or NO2] which are useful for treating or preventing inflammatory and immune cell-mediated diseases (no data) are disclosed as well as methods for their preparation Thus, II was prepared by cyclocondensation of 4-amino-2,6-dichloropyridine with (R)-α-methyl-4-bromophenylalanine Me ester isocyanate and quenched with acetic anhydride. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K031-44
ICS A61K031-675; C07F009-06; C07D401-00; C07D401-04; C07D401-14; C07D413-00; C07D417-04; C07D417-14

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 17 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:78235 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:131534
TITLE: Novel N-aryl nitrogen heterocyclic compounds useful in the treatment of inflammatory disease
INVENTOR(S): ***Kelly, Terence Alfred; Sorcek, Ronald John***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007044	A1	20010201	WO 2000-US17712	20000628
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6353013	B1	20020305	US 2000-605574	20000628

PRIORITY APPLN. INFO.: US 1999-144893P P 19990721
OTHER SOURCE(S): MARPAT 134:131534
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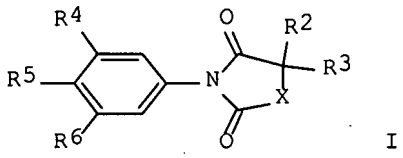

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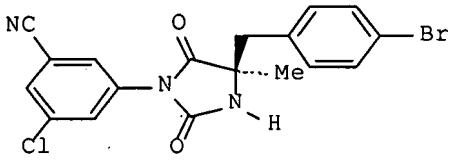


II

AB Novel N-aryl nitrogen heterocyclic compds. I [Y and Z are independently O or S; X = O, S, CHR1, NR1, CHSO2R1 or NSO2R1; R1 = H, (un)substituted branched or unbranched alkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamidino, N-substituted piperidyl, etc.; R2 = H, (un)substituted branched or unbranched alkyl or cycloalkyl; R3 = (CR7R8)x(CR9R10)yR11 where x and y independently = 0 or 1; R7, R8, and R9 independently = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl; R10 = H, OH, alkoxy, acyloxy, branched or unbranched alkyl or cycloalkyl, (un)substituted aryl; R11 = (un)substituted aryl; R4 = Cl, CF3; R5 = H, halo, Me, CF3; R6 = CN or NO2] which are useful for treating or preventing inflammatory and immune cell-mediated diseases (no data) are disclosed as well as methods for their preparation Thus, II was prepared by hydrolysis of 5-(R)-(4-bromobenzyl)-3-(5-acetamino-3-chlorophenyl)-5-methylimidazoline- 2,4-dione followed by Sandmeyer reaction with NaNO2, CuCN and KCN. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K031-4164
ICS A61K031-4166; C07D233-76; C07D233-84; C07D233-86

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 18 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:78178 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:131424
TITLE: Novel indolones and pyrrolopyridinones useful in the treatment of inflammatory disease
INVENTOR(S): ***Kelly, Terence Alfred; Wu, Jiang-Ping***; Kuzmich, Daniel; Ward, Yancey David; Frye, Leah Lynn
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

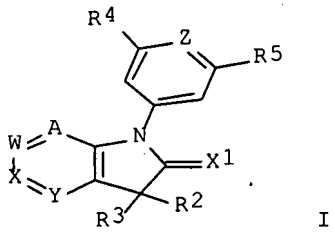
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2001006984	A2	20010201	WO 2000-US17802	20000628
WO 2001006984	A3	20031231		
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2378369	A1	20010201	CA 2000-2378369	20000628
US 6414153	B1	20020702	US 2000-605584	20000628
JP 2004505005	T	20040219	JP 2001-511876	20000628
JP 3833532	B2	20061011		
EP 1399155	A2	20040324	EP 2000-950262	20000628
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				

PRIORITY APPLN. INFO.: US 1999-144895P P 19990721
WO 2000-US17802 W 20000628

OTHER SOURCE(S): MARPAT 134:131424

GI



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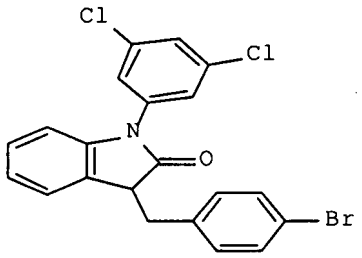

II

AB The title compds. I [A, W, and X independently = N or CH; Y = N, CR1, CSO2R1, CSOR1, CSR1, COR1, CCOR1, CNHR1 where R1 = H, (un)substituted branched or unbranched alkyl or cycloalkyl, alkylcarboxylic acid, alkylphosphonic acid, alkylamindino, etc.; X1 = O, S; R2 = H, (un)substituted branched or unbranched alkyl or cycloalkyl; R3 = (CR6R7)m(CR8R9)nR10 wherein m and n = 0 or 1; R6, R7 and R8 independently = H, OH, alkoxy, acyloxy or (un)substituted branched or unbranched alkyl or cycloalkyl; R9 = R1 or OR1; R10 = (un)substituted aryl; Z = N or CR11 wherein R11 = H, halo, Me or CF3; R4 = Cl or CF3; R5 = H, halo, Me, CN, NO2, CF3 with provision when Z = N or CH, R5 = Cl or CF3] which are useful for treating or preventing inflammatory and immune cell-mediated diseases are disclosed as well as methods for their preparation Thus, II was prepared via Ullman coupling of indole and 1-bromo-3,5-dichlorobenzene, chlorination and hydrolysis to the indolone intermediate, condensation with 4-bromobenzaldehyde and subsequent hydrogenation. II possessed a Kd value > 10 for inhibition of LFA-1 binding to ICAM-1. Pharmaceutical compns. of I suitable for prevention or treatment of inflammatory and immune cell-mediated conditions are disclosed.

IC ICM A61K
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

L23 ANSWER 19 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:332327 ZCAPLUS Full-text
TITLE: Direct transformation of functionalized aromatic/heteroaromatic halides into sulfones.
AUTHOR(S): ***Wu, Jiang-Ping; Emeigh, Jonathan***
CORPORATE SOURCE: Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), ORGN-201. American Chemical Society: Washington, D. C.
CODEN: 69CLAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

AB A direct transformation of functionalized aromatic/hetero-aromatic halides into sulfones is described. This transformation is a three step-one pot procedure which involves 1) generating Grignard reagents from the aromatic/hetero-aromatic halides by magnesium halides exchange; 2) quenching the Grignard reagents with SO2 to produce magnesium sulfinates; 3) alkylating the sulfinate intermediates with alkyl bromides or Michael acceptors. This method avoids oxidation reaction necessary in the conventional sulfone preparation through the oxidation of sulfides and is therefore particularly valuable in the preparation of sulfones where the substrates contain oxidizable groups. In addition a variety of functional groups on the substrates are tolerated.

L23 ANSWER 20 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:612077 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:260456
TITLE: Small molecules useful in the treatment of inflammatory disease
INVENTOR(S): ***Kelly, Terence Alfred***; Bormann, Barbara Jean; Frye, Leah Lynn; ***Wu, Jiang-ping***
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 361 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9839303	A1	19980911	WO 1998-US4254	19980303
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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AU 9865418	A	19980922	AU 1998-65418	19980303
EP 966447	A1	19991229	EP 1998-911475	19980303
EP 966447	B1	20030305		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
EE 9900481	A	20000615	EE 1999-481	19980303
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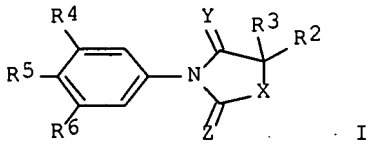
BR 9811260	A	20000808	BR 1998-11260	19980303
HU 200002347	A2	20001028	HU 2000-2347	19980303
JP 2001513821	T	20010904	JP 1998-538772	19980303
AT 233738	T	20030315	AT 1998-911475	19980303
ES 2191286	T3	20030901	ES 1998-911475	19980303
ZA 9807065	A	20000207	ZA 1998-7065	19980806
US 6355664	B1	20020312	US 1999-375010	19990816

MX 9907583	A	20000228	MX 1999-7583		19990817
NO 9904256	A	19991102	NO 1999-4256		19990902
BG 103711	A	20010928	BG 1999-103711		19990902
US 38132	E1	20030603	US 2002-167732		20020612
PRIORITY APPLN. INFO.:			US 1997-40011P	P	19970303
			US 1998-33148	B2	19980302
			WO 1998-US4254	W	19980303
			US 1999-375010	A5	19990816

OTHER SOURCE(S): MARPAT 129:260456
GI



I

AB Title small mols. [I; Y = O, S; Z = O, S; X = CH2, NH, CHSO2H, etc.; R2 = H, cycloalkyl, OH, etc.; R3 = H, OH, alkyloxy, alkyl; R4 = Cl, CF3; R5 = H, F, Cl, Br, I, CH3, CF3; R6 = H, F, Cl, Br, I, CH3, CF3] and pharmaceutically acceptable salts are prepared A method treating or preventing inflammatory and immune cell-mediated diseases by the administration of certain novel and known small mols. such as (R)-I (X = NH; Y = O; Z = O; R2 = CH3; R3 = 4-BrC6H4CH2; R4 = R6 = Cl; R5 = H).

IC ICM C07D233-76
ICS C07D233-78; C07D233-74; C07D233-80; A61K031-415; C07D207-40; C07F009-6506; C07F009-6558; C07D401-10; C07D403-06; C07D409-06; C07D401-04; C07D263-44; C07D233-86; A61K031-675

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 34, 63

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 21 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:187082 ZCAPLUS Full-text
DOCUMENT NUMBER: 126:233098
TITLE: Effect of Structural Modification of Enol-Carboxamide-Type Nonsteroidal Antiinflammatory Drugs on COX-2/COX-1 Selectivity
AUTHOR(S): Lazer, Edward S.; Miao, Clara K.; Cywin, Charles L.; ***Sorcek, Ronald***; Wong, Hin-Chor; Meng, Zhaoxing; Potocki, Ian; Hoermann, MaryAnn; Snow, Roger J.; Tschantz, Matt A.; ***Kelly, Terence A.***; McNeil, Daniel W.; Coutts, Simon J.; Churchill, Laurie; Graham, Anne G.; David, Eva; Grob, Peter M.; Engel, Wolfhard; Meier, Hans; Trummlitz, Guenter
CORPORATE SOURCE: Department of Inflammatory Diseases, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (1997), 40(6), 980-989
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Meloxicam, an NSAID in the enol-carboxamide class, was developed on the basis of its antiinflammatory activity and relative safety in animal models. In subsequent screening in microsomal assays using human COX-1 and COX-2, we discovered that it possessed a selectivity profile for COX-2 superior to piroxicam and other marketed NSAIDs. We therefore embarked on a study of enol-carboxamide type compds. to determine if COX-2 selectivity and potency could be dramatically improved by structural modification. Substitution at the 6- and 7-positions of the 4-oxo-1,2-benzothiazine-3- carboxamide, alteration of the N-Me substituent, and amide modification were all examined In addition we explored several related systems including the isomeric 3-oxo-1,2-benzothiazine-4-carboxamides, thienothiazines, indolothiazines, benzothienothiazines, naphthothiazines, and 1,3- and 1,4-dioxoisoquinolines. While a few examples were found with greater potency in the COX-2 assay, no compound tested had a better COX-2/COX-1 selectivity profile than that of meloxicam.

CC 1-3 (Pharmacology)
Section cross-reference(s): 28

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 22 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:22847 ZCAPLUS Full-text
DOCUMENT NUMBER: 86:22847
TITLE: Charged particle spectra from 100 MeV proton on nickel-58
AUTHOR(S): ***Wu, J. R.***; Chang, C. C.; Holmgren, H. D.; Wall, N. S.; Didelez, J. P.; Butterfield, C.
CORPORATE SOURCE: Dep. Phys., Univ. Maryland, College Park, MD, USA
SOURCE: Clustering Phenom. Nucl., Invited Lect. Contrib. Pap. Int. Conf., 2nd (1975), Issue ORO-4856-26, 360-1. Editor(s): ***Goldberg, D. A.; Marion, J. B.; Wallace, S. J.*** NTIS: Springfield, Va.
CODEN: 34GDA8
DOCUMENT TYPE: Conference
LANGUAGE: English

AB Charged particle spectra resulting from 100-MeV p bombardment of 58Ni [13981-79-8] were measured with a triple-counter-telescope. Data are presented on energy spectra at 9 angles, angle-integrated energy spectra, energy-integrated angular distributions, and angular distributions at different energy intervals. The integral emission cross sections for p (excluding elastic peak), d, t, τ, and α were 890 ± 30, 87 ± 10, 9 ± 3, 13 ± 4, and 120 ± 14 mb, resp. The high-energy angular distributions are anisotropic, indicating preequil. emission, whereas the low-energy distributions are nearly isotropic, suggesting an evaporation process.

CC 70-2 (Nuclear Phenomena)

L23 ANSWER 23 OF 23 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:22837 ZCAPLUS Full-text
DOCUMENT NUMBER: 86:22837
TITLE: Quasifree scattering in the 24Mg(p,pα)20Ne reaction at 100 MeV
AUTHOR(S): Steinberg, R. I.; Chang, C. C.; Chant, N. S.; Didelez, J. P.; Holmgren, H. D.; Roos, Philip G.; ***Wu, J. S.***
CORPORATE SOURCE: Dep. Phys. Astron., Univ. Maryland, College Park, MD, USA
SOURCE: Clustering Phenom. Nucl., Invited Lect. Contrib. Pap. Int. Conf., 2nd (1975), Issue ORO-4856-26, 315-16. Editor(s): ***Goldberg, D. A.; Marion, J. B.; Wallace, S. J.*** NTIS: Springfield, Va.

CODEN: 34GDA8
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Quasifree scattering data are presented for the 24Mg(p,pα)20Ne reaction for 2 pairs of quasifree angles for an incident p energy of 100 MeV.
CC 70-2 (Nuclear Phenomena)

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DICTIONARY FILE UPDATES:  26 JUN 2007  HIGHEST RN 939408-72-7

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FILE LAST UPDATED: 26 Jun 2007  (20070626/ED)

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  substance identification.
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=> d stat que L20
L1              STR
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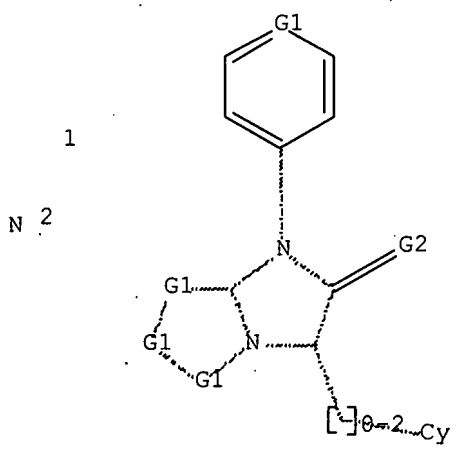

G1 [@1],[@2]
G2 O,S

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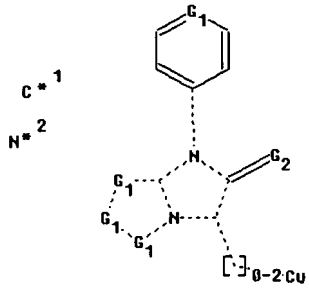

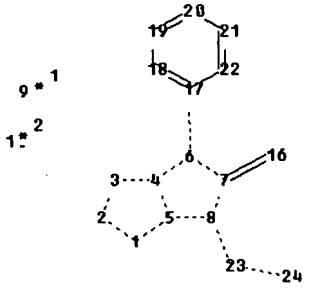

chain nodes :
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ring nodes :
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ring bonds :
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exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 6-17 7-8 7-16 8-23 17-18 17-22 18-19
19-20 20-21 21-22 23-24

G1:[*1],[*2]

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom
Generic attributes :
24:
Saturation : Unsaturated

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L20 28 SEA FILE=ZCAPLUS ABB=ON PLU=ON L19

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L34 21 L20 NOT L23

=> d ibib abs hitstr L34 1-21

L34 ANSWER 1 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1070309 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:389375
TITLE: Derivatives of [6,7-dihydro-5H-imidazo[1,2-alpha]imidazole-3-sulfonyl]-azetidine-carboxylic acids, esters and amides and use thereof as anti-inflammatory agents
INVENTOR(S): Brunette, Steven Richard
PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany; Boehringer Ingelheim Pharma Gmbh & Co. KG
SOURCE: PCT Int. Appl., 52pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006107941	A1	20061012	WO 2006-US12455	20060404

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

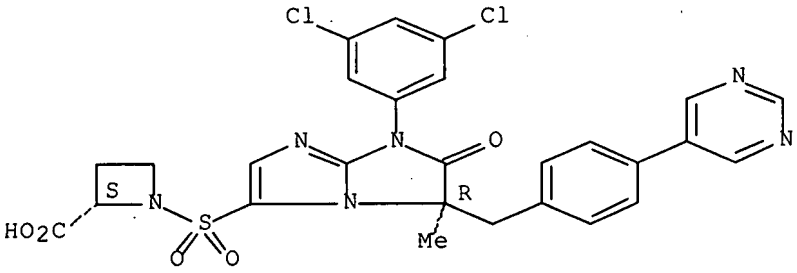
US 2006229287 A1 20061012 US 2006-278579 20060404
PRIORITY APPLN. INFO.: US 2005-668906P P 20050406
OTHER SOURCE(S): MARPAT 145:389375

AB Derivs. of [6,7-dihydro-5H-imidazo[1,2-α]imidazole-3-sulfonyl]- azetidine-carboxylic acids, esters and amides which exhibit good inhibitory effect upon the interaction of cell adhesion mols. (CAMs) and leukointegrins and are thus useful in the treatment of inflammatory disease.

IT ***911634-16-7P 911634-18-9P 911634-19-0P***
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(derivs. of [dihydro-5H-imidazoimidazolesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)

RN 911634-16-7 ZCAPLUS
CN 2-Azetidinecarboxylic acid, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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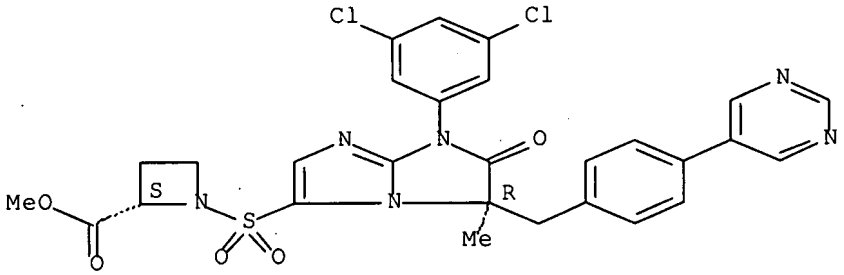
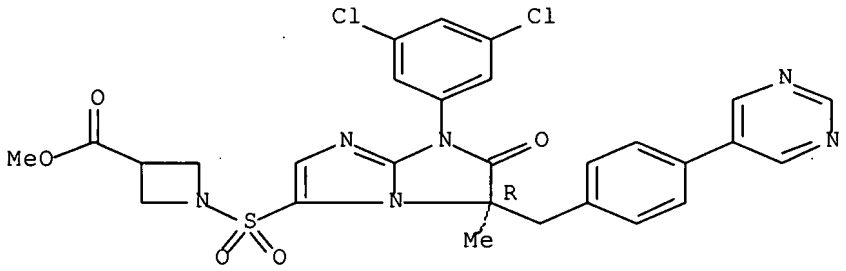
CN 2-Azetidinecarboxylic acid, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 911634-19-0 ZCAPLUS
CN 3-Azetidinecarboxylic acid, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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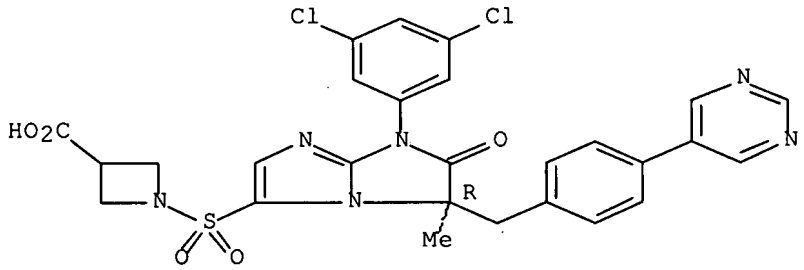
911634-23-6P 911634-24-7P 911634-25-8P
911634-26-9P 911634-27-0P 911634-28-1P
911634-29-2P 911634-30-5P 911634-31-6P
911634-32-7P 911634-33-8P 911634-34-9P
911634-35-0P 911634-36-1P 911634-37-2P
911634-38-3P 911634-39-4P 911634-40-7P
911634-41-8P 911634-44-1P 911634-45-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(derivs. of [dihydro-5H-imidazoimidazolesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)

RN 911634-20-3 ZCAPLUS

CN 3-Azetidinecarboxylic acid, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

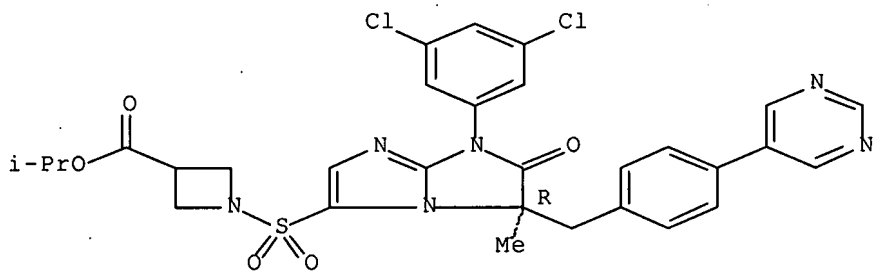
Absolute stereochemistry.



RN 911634-21-4 ZCAPLUS

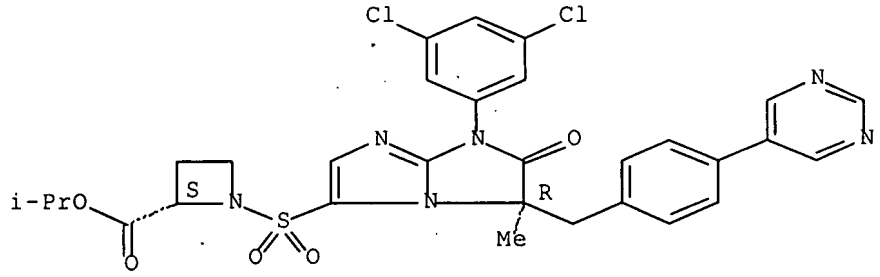
CN 3-Azetidinecarboxylic acid, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



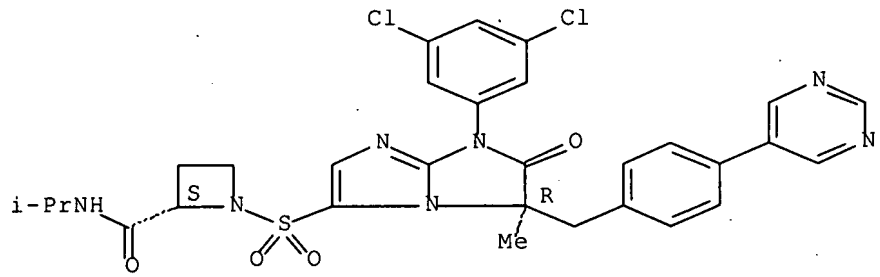
RN 911634-22-5 ZCAPLUS
CN 2-Azetidinecarboxylic acid, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, 1-methylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



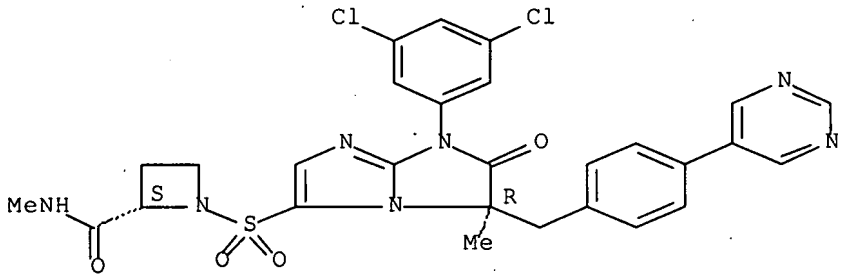
RN 911634-23-6 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



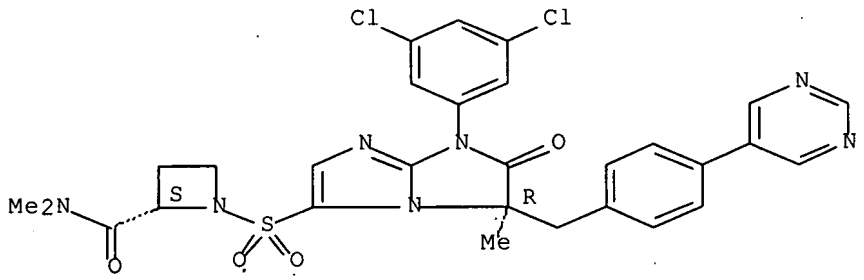
RN 911634-24-7 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



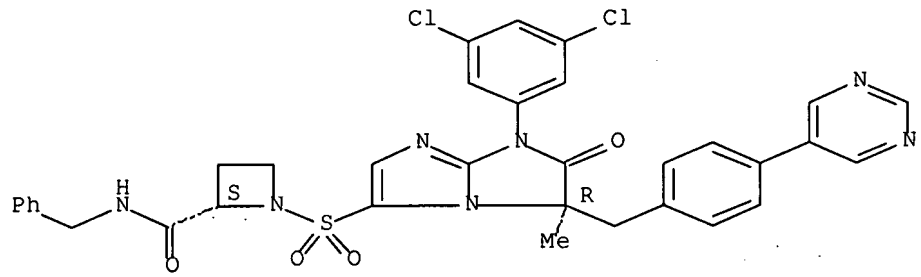
RN 911634-25-8 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N,N-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 911634-26-9 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(phenylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

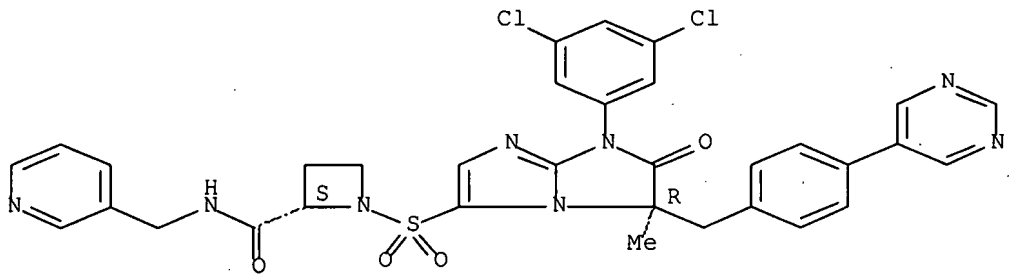
Absolute stereochemistry.



RN 911634-27-0 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-

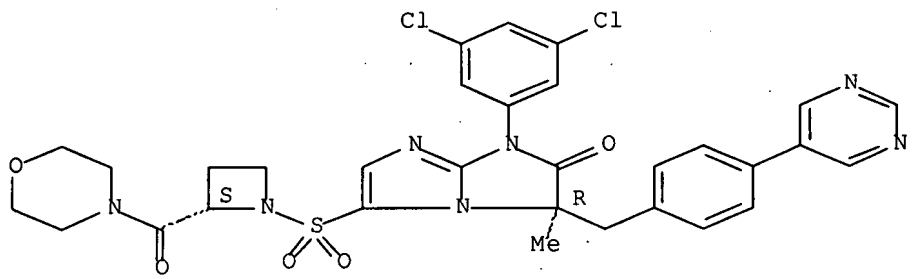
5-yl]sulfonyl]-N-(3-pyridinylmethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



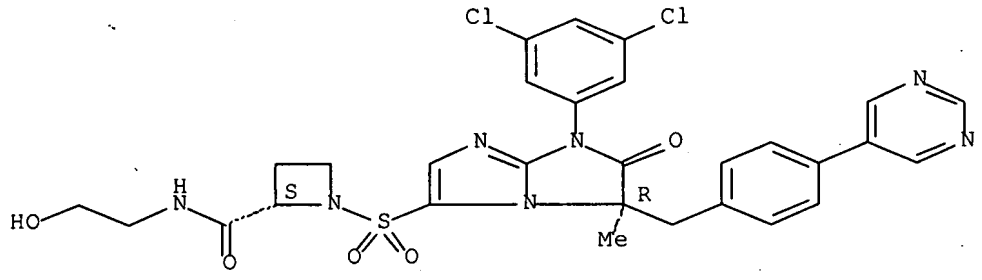
RN 911634-28-1 ZCAPLUS
CN Morpholine, 4-[[(2S)-1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-2-azetidinyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 911634-29-2 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(2-hydroxyethyl)-, (2S)- (9CI) (CA INDEX NAME)

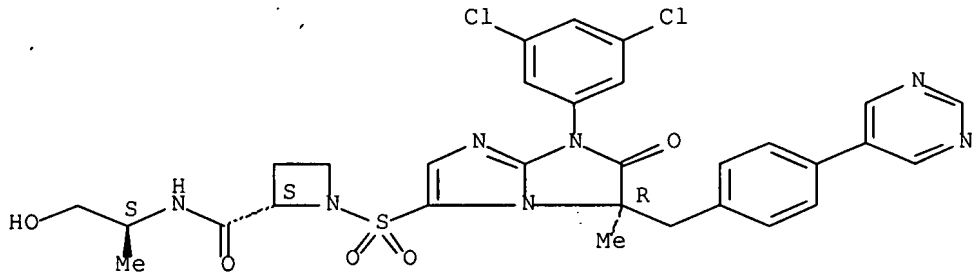
Absolute stereochemistry.



RN 911634-30-5 ZCAPLUS

CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-[(1S)-2-hydroxy-1-methylethyl]-, (2S)- (9CI) (CA INDEX NAME)

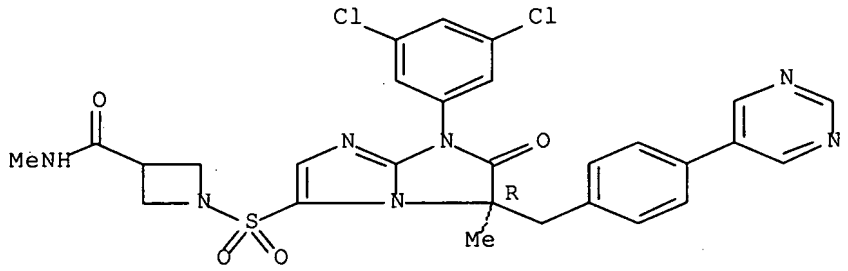
Absolute stereochemistry.



RN 911634-31-6 ZCAPLUS

CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-methyl- (9CI) (CA INDEX NAME)

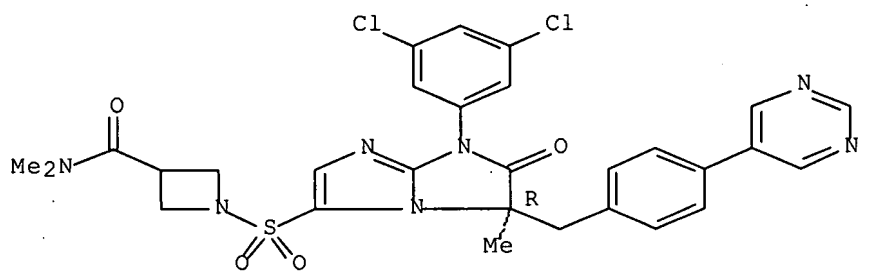
Absolute stereochemistry.



RN 911634-32-7 ZCAPLUS

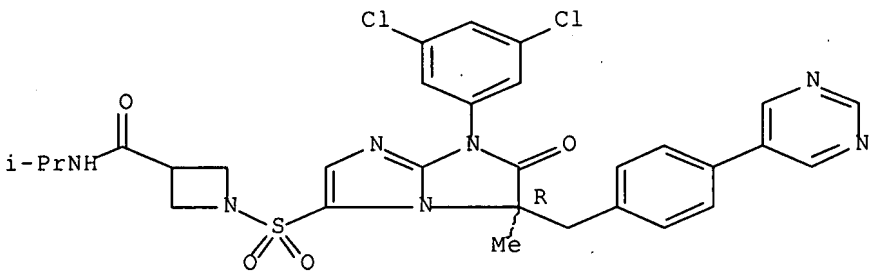
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



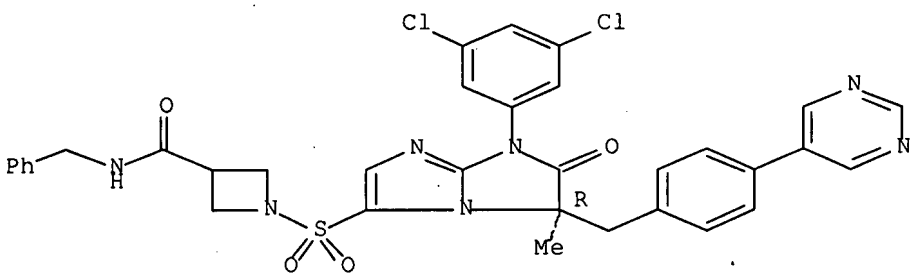
RN 911634-33-8 ZCAPLUS
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



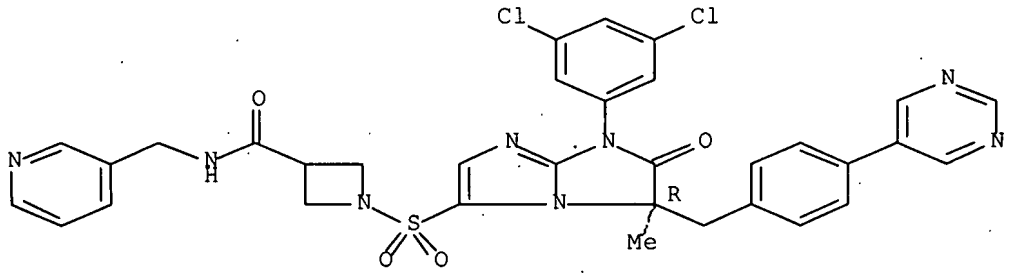
RN 911634-34-9 ZCAPLUS
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



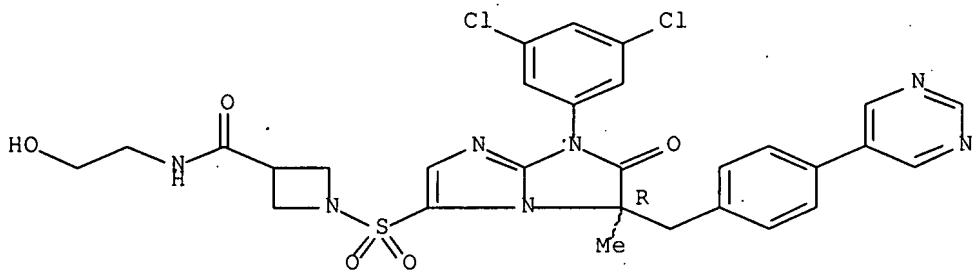
RN 911634-35-0 ZCAPLUS
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



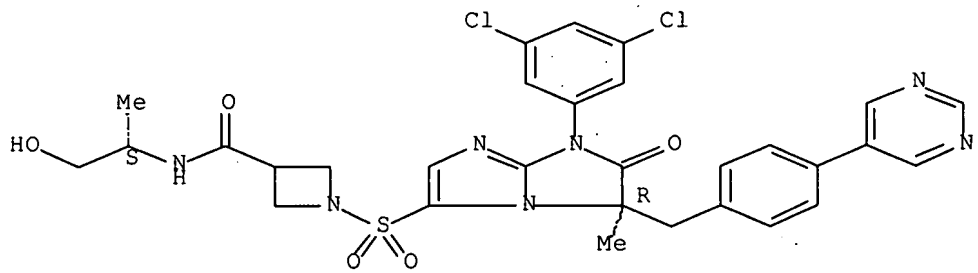
RN 911634-36-1 ZCAPLUS
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



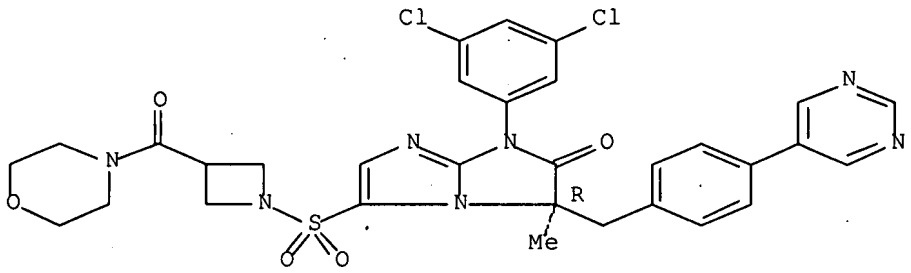
RN 911634-37-2 ZCAPLUS
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-N-[(1S)-2-hydroxy-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



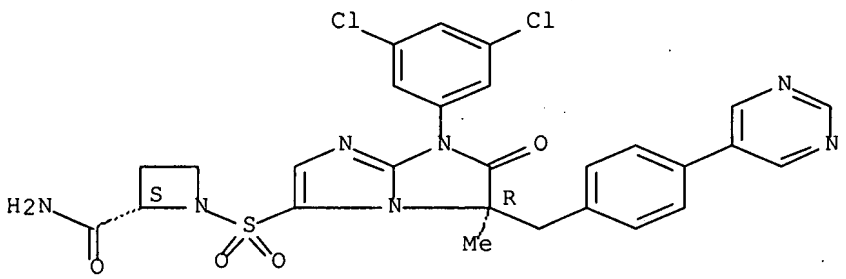
RN 911634-38-3 ZCAPLUS
CN Morpholine, 4-[[1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-3-azetidinyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



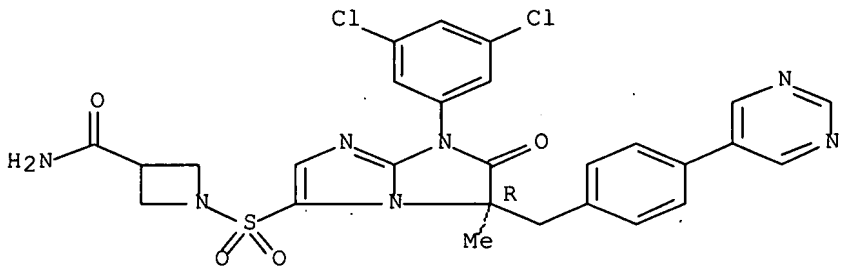
RN 911634-39-4 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 911634-40-7 ZCAPLUS
CN 3-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

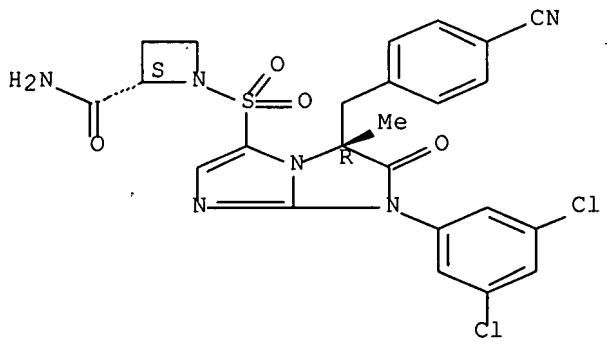
Absolute stereochemistry.



RN 911634-41-8 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-

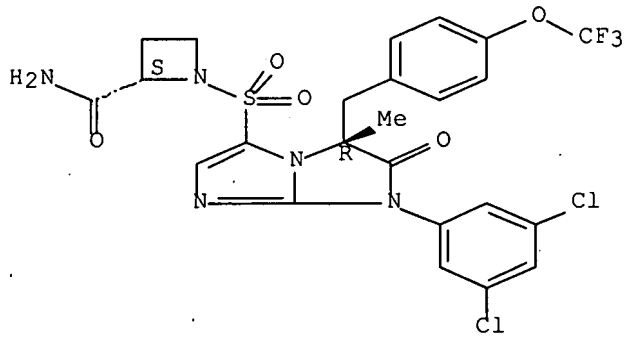
yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



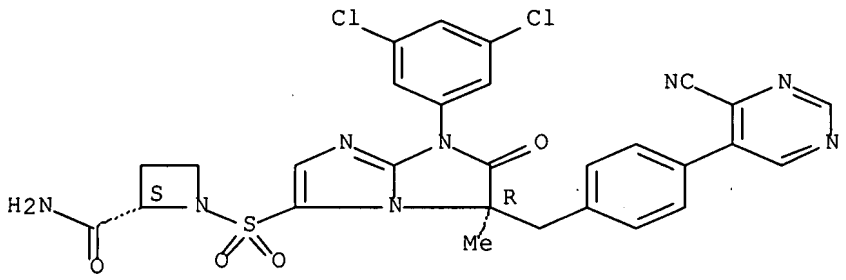
RN 911634-44-1 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(trifluoromethoxy)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



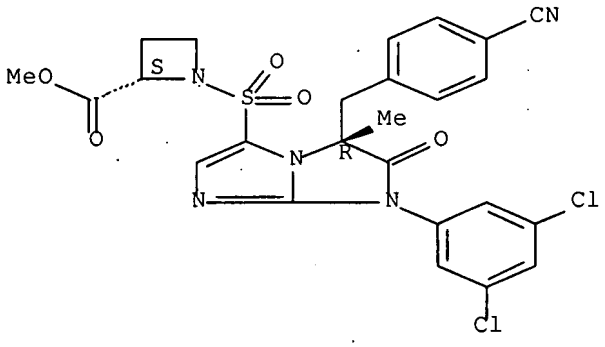
RN 911634-45-2 ZCAPLUS
CN 2-Azetidinecarboxamide, 1-[[(3R)-3-[[4-(4-cyano-5-pyrimidinyl)phenyl]methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



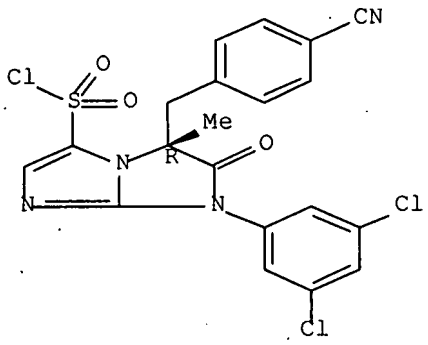
IT ***911634-42-9P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; derivs. of [dihydro-5H-imidazoimidazolesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)
RN 911634-42-9 ZCAPLUS
CN 2-Azetidinecarboxylic acid, 1-[[(3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



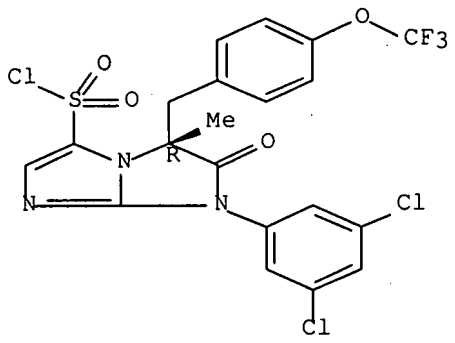
IT ***688756-08-3***, (R)-5-(4-Cyanobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride ***688756-19-6***, (R)-7-(3,5-Dichlorophenyl)-5-methyl-6-oxo-5-(4-trifluoromethoxybenzyl)-6,7-dihydro-5H-imidazo[1,2-a]imidazole-3-sulfonyl chloride ***911634-17-8*** ***911634-43-0***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; derivs. of [dihydro-5H-imidazoimidazolesulfonyl]-azetidine-carboxylic acids, esters and amides as anti-inflammatory agents and inhibition of cell adhesion mols. interaction with leukointegrins)
RN 688756-08-3 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



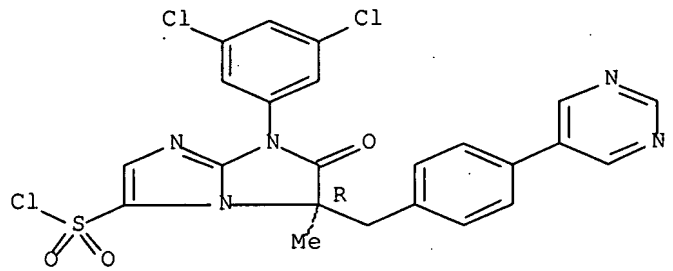
RN 688756-19-6 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(trifluoromethoxy)phenyl]methyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 911634-17-8 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

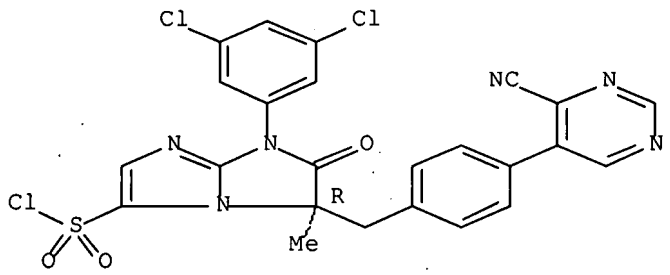
Absolute stereochemistry.



RN 911634-43-0 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-5-sulfonyl chloride, 3-[[4-(4-cyano-5-pyrimidinyl)phenyl]methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

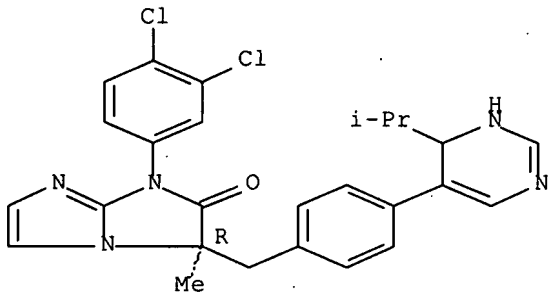
L34 ANSWER 2 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:600124 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:230586
TITLE: Mild Iodine-Magnesium Exchange of Iodoaromatics Bearing a Pyrimidine Ring with Isopropylmagnesium Chloride
AUTHOR(S): Wang, Xiao-Jun; Xu, Yibo; Zhang, Li; Krishnamurthy, Dhileepkumar; Senanayake, Chris H.
CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Organic Letters (2006), 8(14), 3141-3144
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:230586

AB (Iodo)arenes bearing a reactive pyrimidine ring underwent a clean iodine-magnesium exchange with isopropylmagnesium chloride in the presence of bis[2-(dimethylamino)ethyl] ether to provide the corresponding Grignard reagents. The presence of bis[2-(dimethylamino)ethyl] ether prevented reduction of the pyrimidine ring and addition by isopropylmagnesium chloride. As a result, the newly formed reactive Grignard reagents were allowed to react with electrophiles in a highly selective manner to afford adducts in excellent yields.

IT ***905840-79-1P 905840-80-4P 905840-81-5P***
RL: BYP (Byproduct); PREP (Preparation)
(mild iodine-magnesium exchange of chiral iodo(chlorophenyl)methyl[(pyrimidinyl)phenyl]methyl]imidazo[1,2-a]imidazolone derivs. with isopropylmagnesium chloride)

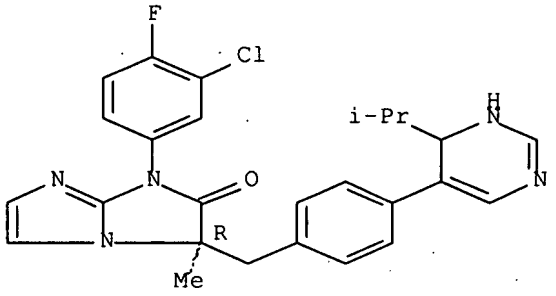
RN 905840-79-1 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-[[4-[1,4-dihydro-4-(1-methylethyl)-5-pyrimidinyl]phenyl]methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



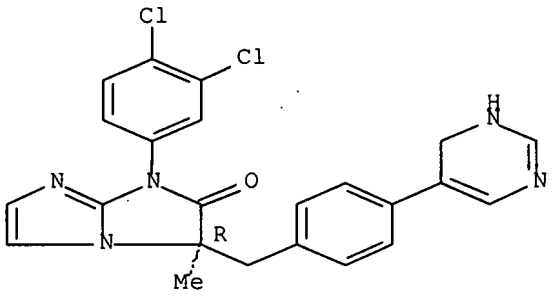
RN 905840-80-4 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3-chloro-4-fluorophenyl)-3-[[4-[1,4-dihydro-4-(1-methylethyl)-5-pyrimidinyl]phenyl]methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 905840-81-5 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-[[4-(1,4-dihydro-5-pyrimidinyl)phenyl]methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



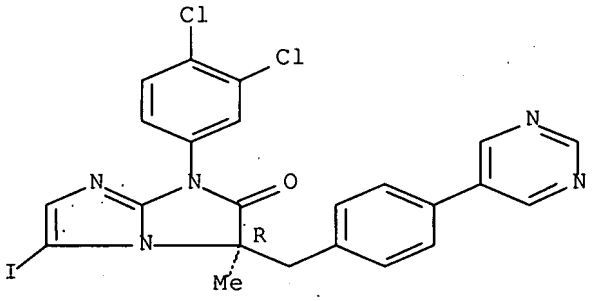
IT *905840-75-7P 905840-76-8P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(mild iodine-magnesium exchange of chiral iodo(chlorophenyl)methyl[(pyrimidinyl)phenyl]methyl]imidazo[1,2-a]imidazolone derivs. with isopropylmagnesium chloride)

RN 905840-75-7 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-5-iodo-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

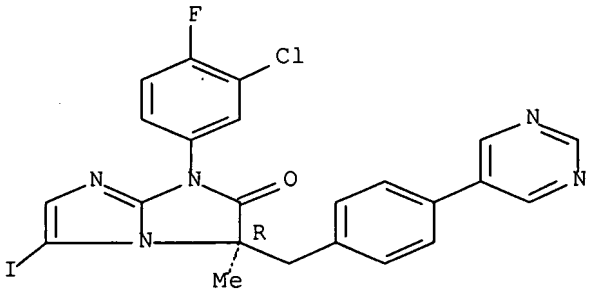
Absolute stereochemistry.



RN 905840-76-8 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3-chloro-4-fluorophenyl)-5-iodo-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



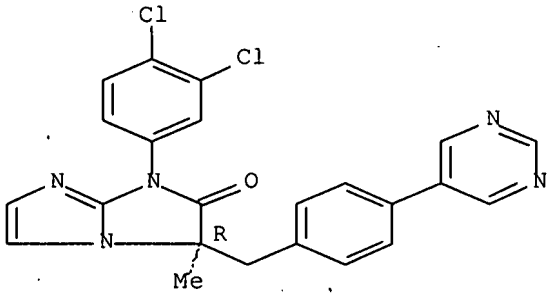
IT *905840-77-9P 905840-78-0P*

RL: SPN (Synthetic preparation); PREP (Preparation)
(mild iodine-magnesium exchange of chiral iodo(chlorophenyl)methyl[(pyrimidinyl)phenyl]methyl]imidazo[1,2-a]imidazolone derivs. with isopropylmagnesium chloride)

RN 905840-77-9 ZCAPLUS

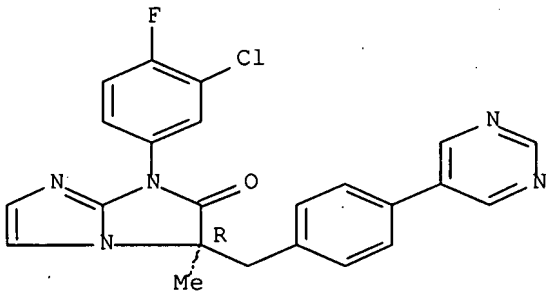
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



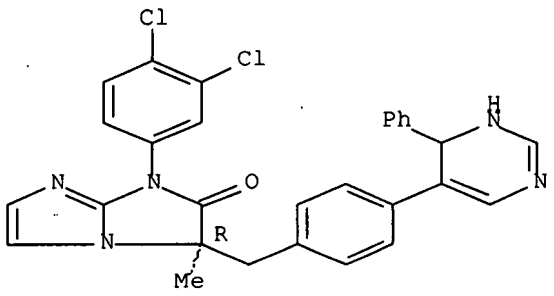
RN 905840-78-0 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3-chloro-4-fluorophenyl)-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT *905840-85-9P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of chiral iodo(chlorophenyl)methyl[(pyrimidinyl)phenyl]methyl]imidazo[1,2-a]imidazolone with phenylmagnesium chloride)
RN 905840-85-9 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,4-dichlorophenyl)-3-[[4-(1,4-dihydro-4-phenyl-5-pyrimidinyl)phenyl]methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:104683 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:192252
TITLE: Process for preparation of oxoimidazoimidazolesulfonamides.
INVENTOR(S): Wang, Xiao-Jun; Wirth, Thomas; Nicola, Thomas; Zhang, Li; Frutos, Rogelio Perez; Xu, Yibo; Krishnamurihy, Dhileopkumar; Nummy, Laurence John; Varsolona, Richard J.; Senanayake, Chris Hugh; Kroeber, Jutta
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim International G.m.b.H.
SOURCE: U.S. Pat. Appl. Publ., 24 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006025447	A1	20060202	US 2005-188377	20050725
AU 2005269634	A1	20060209	AU 2005-269634	20050725
CA 2573398	A1	20060209	CA 2005-2573398	20050725
WO 2006014828	A1	20060209	WO 2005-US26148	20050725
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1776367	A1	20070425	EP 2005-775277	20050725
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BA, HR, YU				
IN 2007DN00045	A	20070427	IN 2007-DN45	20070102
PRIORITY APPLN. INFO.:			US 2004-591398P P	20040727
			WO 2005-US26148 W	20050725

OTHER SOURCE(S): CASREACT 144:192252; MARPAT 144:192252
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

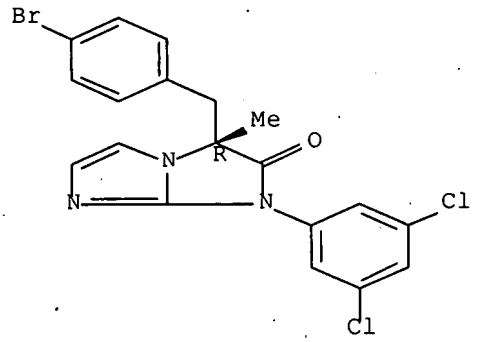
AB Title compds. [I; R1 = Br, F3CO, cyano, (amino-substituted) pyrimidin-5-yl; Q = R2R3NSO2; .R2, R3 = H, (substituted) alkyl; R2R3N = (substituted) pyrrolidinyl, piperidinyl], were prepared by treatment of I (R1 as above; Q = halo) with an alkylmagnesium halide, SO2, N-chlorosuccinimide, and R2R3NH. Thus, title compound (II) was prepared in 75% yield by treatment of the

corresponding iodide with isopropylmagnesium chloride/tetramethylethylenediamine/SO2/N-chlorosuccinimide/isonipecotamide/diisopropylethylamine in THF at -20° to 22°.

IT ***321656-72-8P 321656-73-9P 321720-72-3P 321722-94-5P 875210-71-2P 875210-72-3P 875210-76-7P 875210-77-8P***
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparation of dihydrooxoimidazoimidazolesulfonamides)

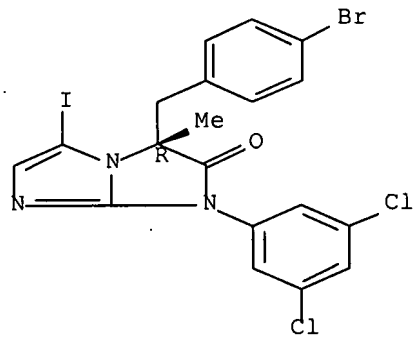
RN 321656-72-8 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



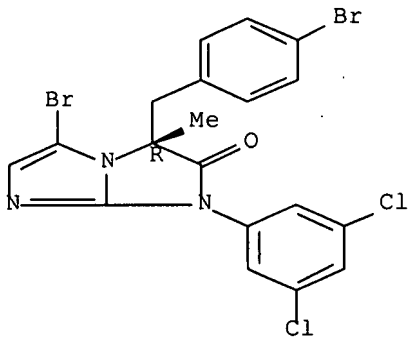
RN 321656-73-9 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



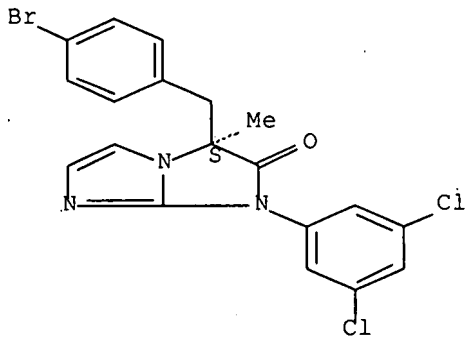
RN 321720-72-3 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 5-bromo-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



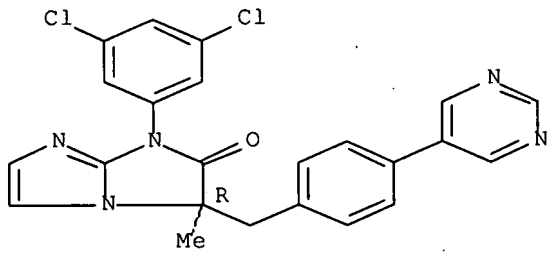
RN 321722-94-5 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



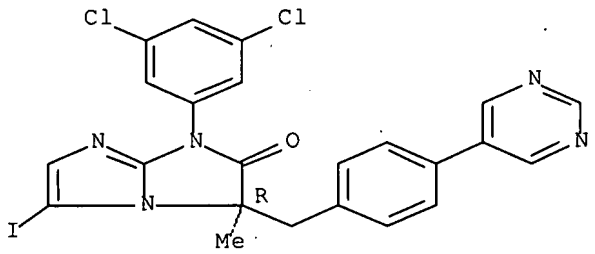
RN 875210-71-2 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



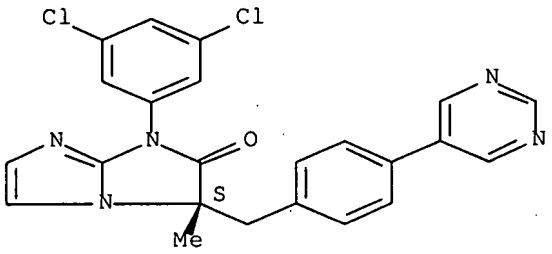
RN 875210-72-3 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-5-iodo-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



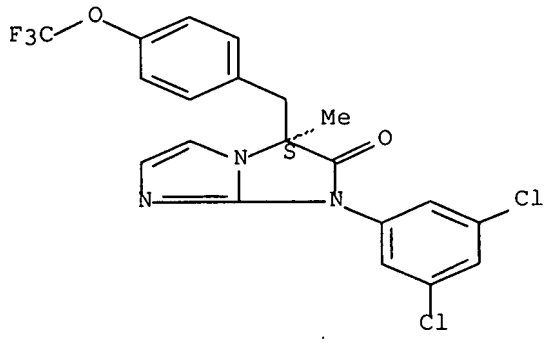
RN 875210-76-7 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-methyl-3-[[4-(5-pyrimidinyl)phenyl]methyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 875210-77-8 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 1-(3,5-dichlorophenyl)-3-methyl-3-[[4-(trifluoromethoxy)phenyl]methyl]-, (3S)- (9CI) (CA INDEX NAME)

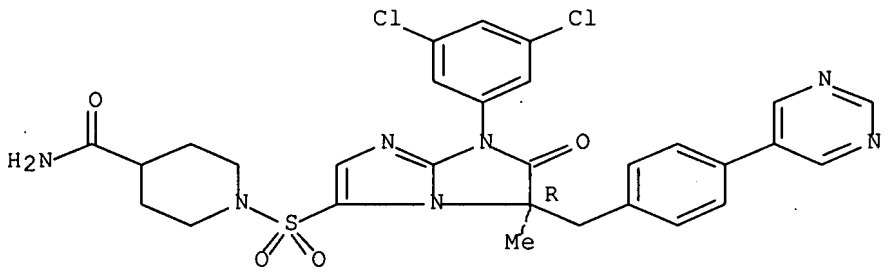
Absolute stereochemistry.



IT *321656-57-9P 321656-61-5P 321718-99-4P*
688756-00-5P 875210-67-6P 875210-75-6P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of dihydrooxoimidazoimidazolesulfonamides)

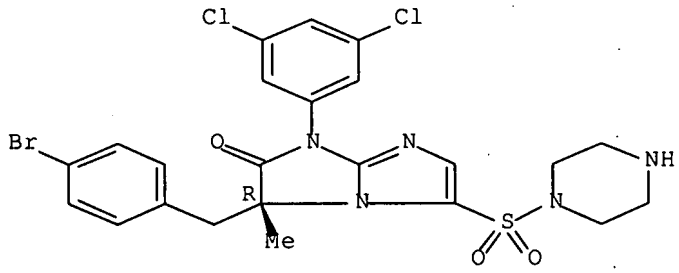
RN 321656-57-9 ZCAPLUS
CN 4-Piperidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



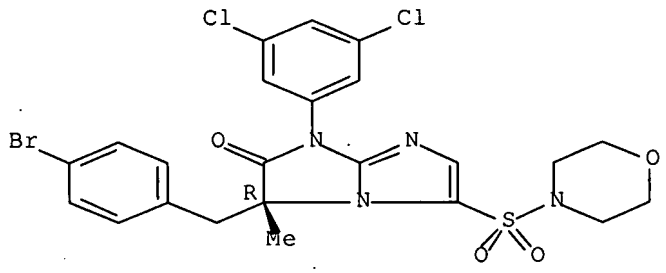
RN 321656-61-5 ZCAPLUS
CN Piperazine, 1-[[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



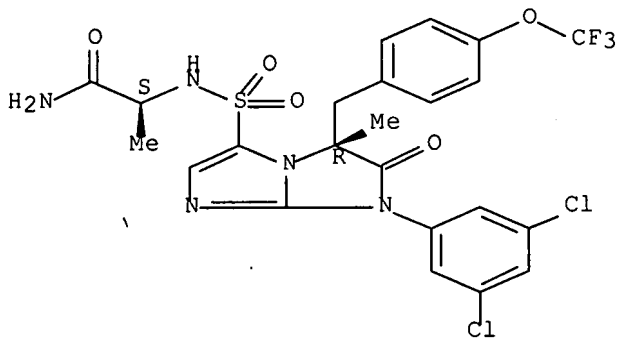
RN 321718-99-4 ZCAPLUS
CN Morpholine, 4-[[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



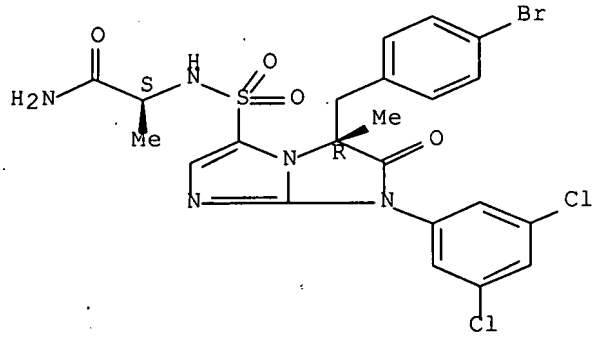
RN 688756-00-5 ZCAPLUS
CN Propanamide, 2-[[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(trifluoromethoxy)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



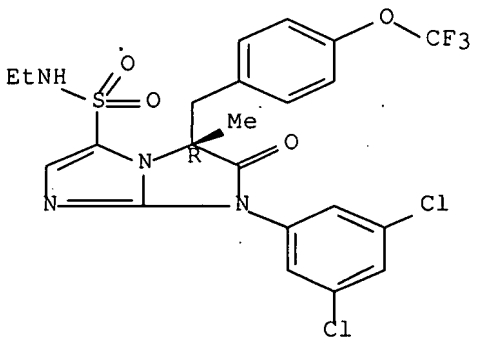
RN 875210-67-6 ZCAPLUS
CN Propanamide, 2-[[[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 875210-75-6 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-5-sulfonamide, 1-(3,5-dichlorophenyl)-N-ethyl-2,3-dihydro-3-methyl-2-oxo-3-[[4-(trifluoromethoxy)phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 4 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:177881 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:274025
TITLE: Methods using a combination of a p38 MAP kinase inhibitor with another active agent for the treatment of chronic obstructive pulmonary disease (COPD) and pulmonary hypertension
INVENTOR(S): Gupta, Abhya; Iacono, Philippe Didier; Kelash-Cannavo, Linda Jean; Madwed, Jeffrey B.; Park, Jung-Yong; Way, Susan Lynn; Yazdanian, Mehran
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim Pharma GmbH & Co. KG; Boehringer Ingelheim France S.A.S.
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005018624	A2	20050303	WO 2004-US27013	20040819
WO 2005018624	A3	20050506		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004266719	A1	20050303	AU 2004-266719	20040819
CA 2536293	A1	20050303	CA 2004-2536293	20040819
US 2005148555	A1	20050707	US 2004-921448	20040819
EP 1658060	A2	20060524	EP 2004-781654	20040819
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1838958	A	20060927	CN 2004-80024151	20040819
BR 2004013757	A	20061031	BR 2004-13757	20040819

JP 2007503393 T 20070222 JP 2006-524065 20040819
PRIORITY APPLN. INFO.: US 2003-497376P P 20030822
WO 2004-US27013 W 20040819

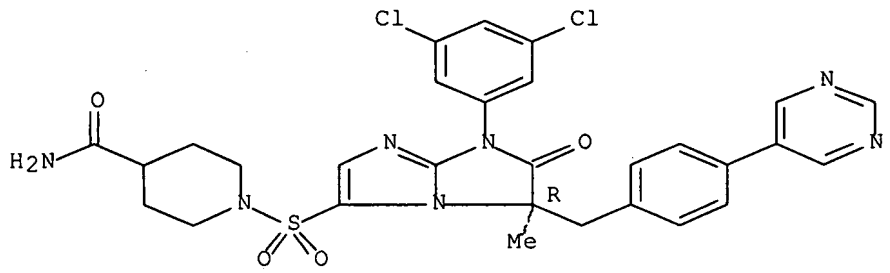
AB Methods are disclosed for treating COPD and pulmonary hypertension using p38 MAP Kinase inhibitors in combination with one or more other active ingredients.

IT ***321656-57-9***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(p38 MAP kinase inhibitor combination with another active agent for treatment of chronic obstructive pulmonary disease and pulmonary hypertension)

RN 321656-57-9 ZCAPLUS

CN 4-Piperidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 5 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:41390 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:299796
TITLE: Development of a Scalable Process for 1-(3,5-Dichlorophenyl)-5-iodo-3-methyl-(4-methylbenzyl)-1H-imidazo[1,2-a]imidazol-2-one: A Key Intermediate for the Synthesis of LFA-1 Inhibitors
AUTHOR(S): Frutos, Rogelio P.; Eriksson, Magnus; Wang, Xiao-Jun; Byrne, Denis; Varsolona, Richard; Johnson, Michael D.; Nummy, Lawrence; Krishnamurthy, Dhileepkumar; Senanayake, Chris H.
CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT, 06877-0368, USA
SOURCE: Organic Process Research & Development (2005), 9(2), 137-140
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:299796

AB A safe, robust, chromatog.-free and reproducible process for the multi-kilogram synthesis of 3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-5- iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one, a key intermediate for the synthesis of LFA-1 inhibitors, was developed and implemented at pilot plant scale. The process allowed support of preclin. activities in the LFA-1 program. Major

improvements were realized by lowering the reaction temperature to -15° and changing the solvent from dichloromethane to acetonitrile, and using TMSI/NaI as reagent system for regioselective hydroiodination. Under the improved conditions, the HI catalyzed proto-deiodination pathway of the intermediate was minimized and the intermediate was obtained in high yield and with low impurity profile.

IT ***397329-88-3P 397329-89-4P***

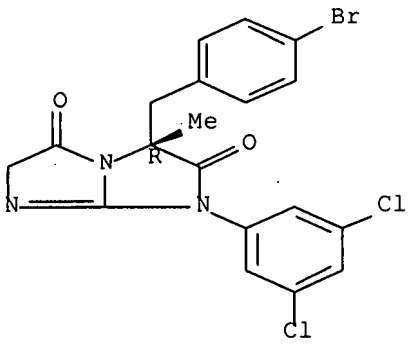
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; pilot-scale process for preparation of dichlorophenyliodo-methylbenzylimidazoimidazolone key intermediate for synthesis of LFA-1 inhibitors)

RN 397329-88-3 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

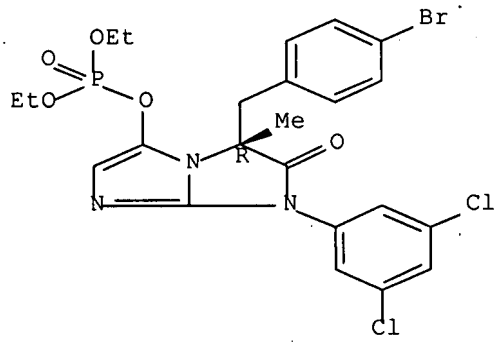
Absolute stereochemistry.



RN 397329-89-4 ZCAPLUS

CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT ***321656-73-9P***

RL: IMF (Industrial manufacture); PREP (Preparation)

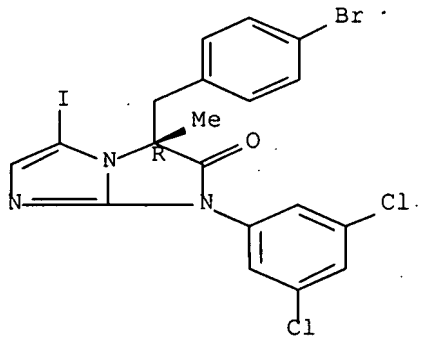
(pilot-scale process for preparation of dichlorophenyliodo-

methylbenzylimidazoimidazolone key intermediate for synthesis of LFA-1 inhibitors)

RN 321656-73-9 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 6 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:39714 ZCAPLUS Full-text

DOCUMENT NUMBER: 143:386961

TITLE: A practical synthesis of highly functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-diones, key intermediates for LFA-1 inhibitors. [Erratum to document cited in CA142:197976]

AUTHOR(S): Wang, Xiao-jun; Xu, Yibo; Zhang, Li; Krishnamurthy, Dhileepkumar; Nummy, Laurence; Farina, Vittorio; Senanayake, Chris H.

CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

SOURCE: Synlett (2005), (1), 186
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

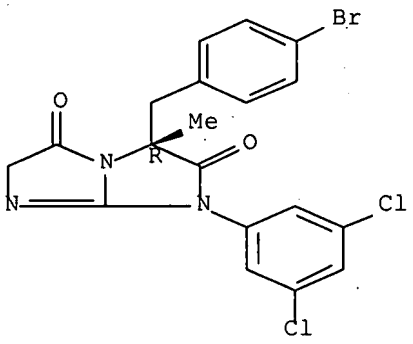
AB The structures of compound 7 in Scheme 1 and compound 9 in Scheme 4 were incorrectly shown; the corrected Schemes 1 and 4 are given.

IT ***397329-88-3P 839678-17-0P 839678-18-1P 839678-19-2P 839678-20-5P 839678-21-6P 839678-22-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-diones as key intermediates for LFA-1 inhibitors (Erratum))

RN 397329-88-3 ZCAPLUS

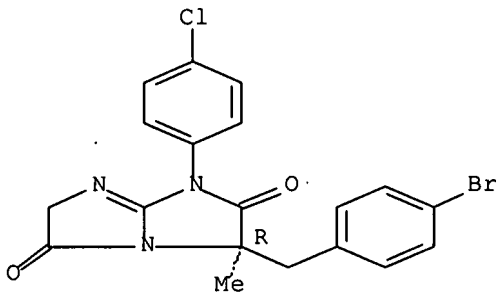
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



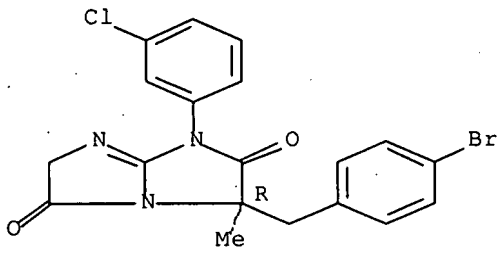
RN 839678-17-0 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



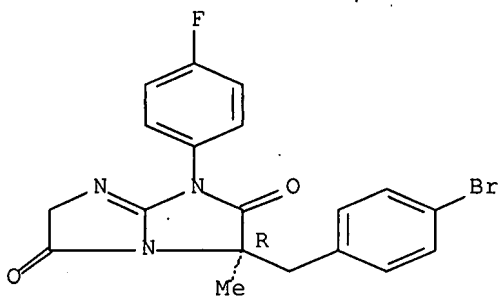
RN 839678-18-1 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



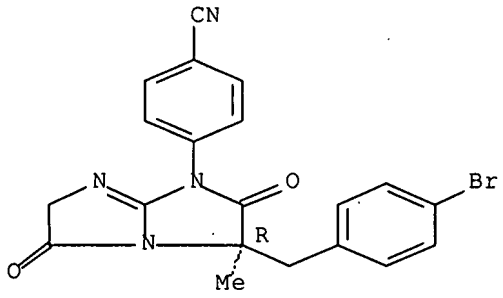
RN 839678-19-2 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-fluorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



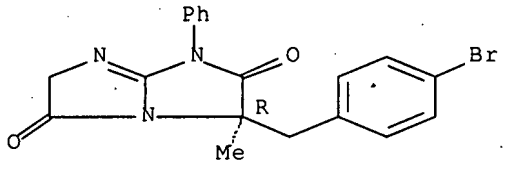
RN 839678-20-5 ZCAPLUS
CN Benzonitrile, 4-[(3R)-3-[(4-bromophenyl)methyl]-2,3,5,6-tetrahydro-3-methyl-2,5-dioxo-1H-imidazo[1,2-a]imidazol-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



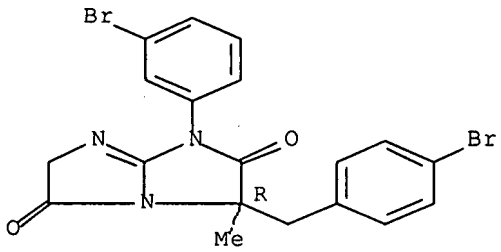
RN 839678-21-6 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-3-methyl-1-phenyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

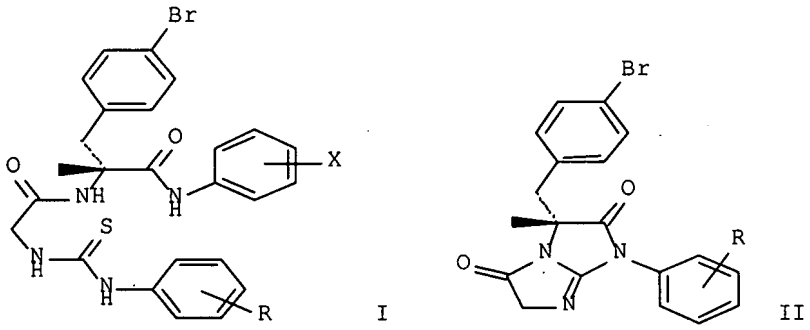


RN 839678-22-7 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 1-(3-bromophenyl)-3-[(4-bromophenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 7 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1128066 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:197976
TITLE: A practical synthesis of highly functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-diones, key intermediates for LFA-1 inhibitors
AUTHOR(S): Wang, Xiao-jun; Xu, Yibo; Zhang, Li; Krishnamurthy, Dhileepkumar; Nummy, Laurence; Farina, Vittorio; Senanayake, Chris H.
CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Synlett (2004), (15), 2800-2802
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:197976
GI



I II

AB An alternative and chromatog.-free approach for synthesis of a new class of LFA-1 inhibitors was developed. A key feature of this process involved a transformation of thioureas I (X = 3,5-Cl2, 4-Cl; R = 4-Cl, H, 3-Cl, etc.) to acyclic guanidine derivs., followed by intramol. cyclization to highly functionalized bicyclic guanidines II, that were subsequently converted to 1H-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors.

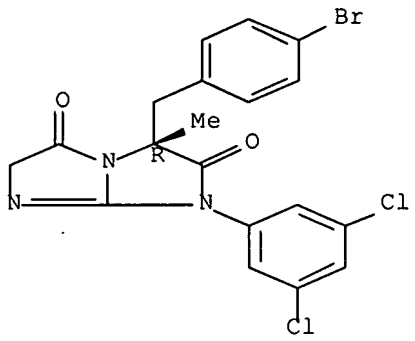
IT *397329-88-3P 839678-17-0P 839678-18-1P 839678-19-2P 839678-20-5P 839678-21-6P 839678-22-7P*

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized fused 1,6-dihydroimidazo[1,2-a]imidazole-2,5-
diones as key intermediates for LFA-1 inhibitors)

RN 397329-88-3 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

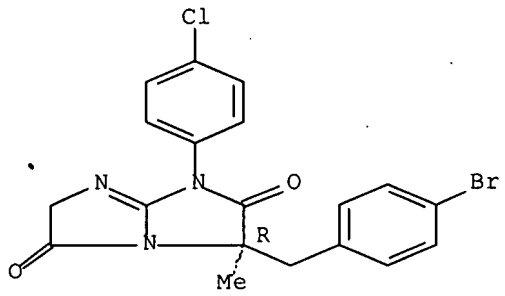
Absolute stereochemistry.



RN 839678-17-0 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

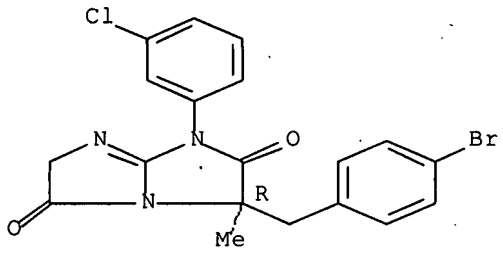
Absolute stereochemistry.



RN 839678-18-1 ZCAPLUS

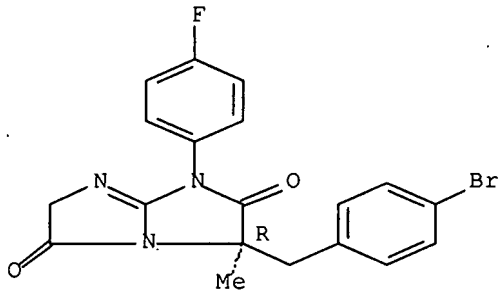
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3-chlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



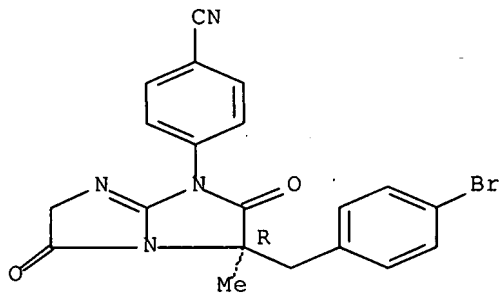
RN 839678-19-2 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(4-fluorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



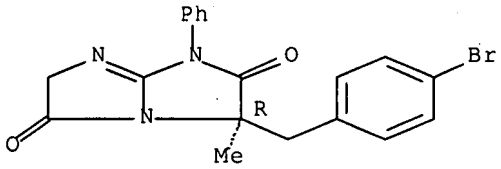
RN 839678-20-5 ZCAPLUS
CN Benzonitrile, 4-[(3R)-3-[(4-bromophenyl)methyl]-2,3,5,6-tetrahydro-3-methyl-2,5-dioxo-1H-imidazo[1,2-a]imidazol-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



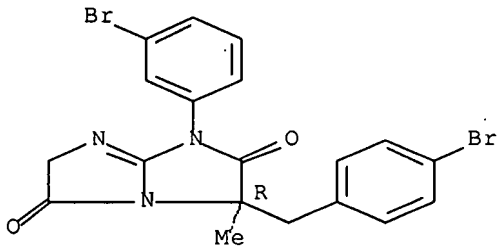
RN 839678-21-6 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-3-methyl-1-phenyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



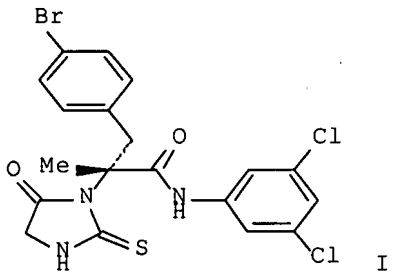
RN 839678-22-7 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 1-(3-bromophenyl)-3-[(4-bromophenyl)methyl]-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

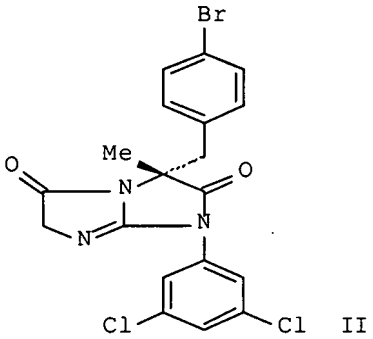


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 8 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1068436 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:197972
TITLE: A practical synthesis of LFA-1 inhibitors utilizing CuCl-promoted intramolecular cyclization of thiohydantoins
AUTHOR(S): Wang, Xiao-jun; Zhang, Li; Xu, Yibo; Krishnamurthy, Dhileepkumar; Varsolona, Richard; Nummy, Laurence; Shen, Sherry; Frutos, Rogelio P.; Byrne, Denis; Chung, J. C.; Farina, Vittorio; Senanayake, Chris H.
CORPORATE SOURCE: Chemical Development Department, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877-0368, USA
SOURCE: Tetrahedron Letters (2005), 46(2), 273-276
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:197972
GI



I



II

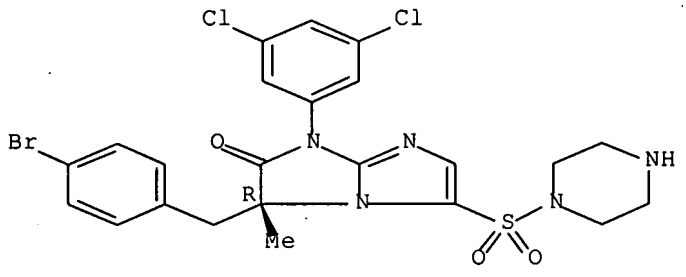
AB An efficient and chromatog.-free approach for synthesis of a new class of LFA-1 (antigen) inhibitors was developed. These compds. are potential inflammation inhibitors (no data). A copper(I) chloride-promoted intramol. cyclization of thiohydantoins serves as a key step to highly functionalized bicyclic guanidines, that were subsequently converted to 1H-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors. This process has been successfully implemented in the pilot plant to produce multi-kilogram quantities of 1H-imidazo[1,2-a]imidazol-2-one LFA-1 inhibitors. The copper chloride (CuCl)-mediated cyclization of a thiourea derivative (I) gave (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-1H- imidazo[1,2-a]imidazole-2,5(3H,6H)-dione (II) in 85-92% yield.

IT ***321656-61-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [[(R)-
[(bromophenyl)methyl][di(chloro)phenyl]dihydro(methyl)
(oxo)imidazo[1,2-a]imidazolyl]sulfonyl]piperazine (bicyclic guanidine) using copper chloride-promoted cyclization of thiourea derivative as key synthetic step)

RN 321656-61-5 ZCAPLUS

CN Piperazine, 1-[[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



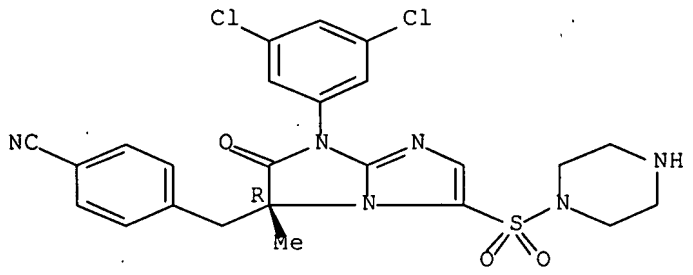
IT ***321656-62-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [[(R)-
[di(chloro)phenyl]dihydro(methyl)(oxo)[(piperazinyl)su
lfonyl]imidazo[1,2-a]imidazolyl]methyl]benzonitrile (bicyclic

guanidine) using copper chloride-promoted cyclization of thiourea derivative as key synthetic step)

RN 321656-62-6 ZCAPLUS

CN Piperazine, 1-[[(3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

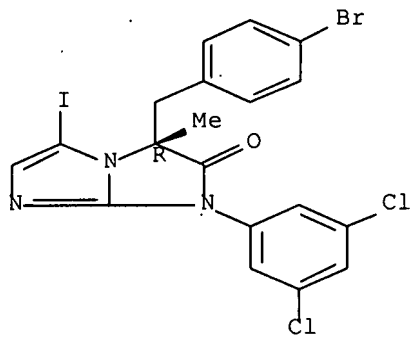


IT *321656-73-9P 321724-08-7P 397329-88-3P*
397329-89-4P 835917-16-3P 835917-17-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of [di(chloro)phenyl](methyl)imidazo[1,2-a]imidazoledione (bicyclic guanidine) using copper chloride-promoted cyclization of N-[di(chloro)phenyl](oxo)(thioxo)imidazolidineethanamide (thiourea derivative) as key synthetic step)

RN 321656-73-9 ZCAPLUS

CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

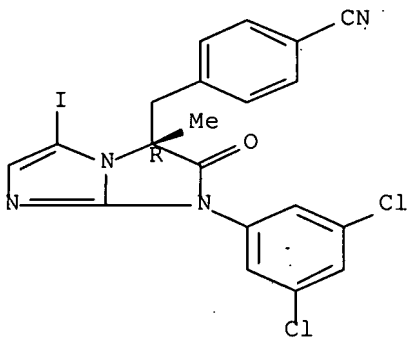
Absolute stereochemistry.



RN 321724-08-7 ZCAPLUS

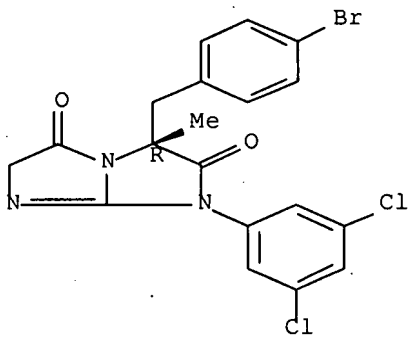
CN Benzonitrile, 4-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-5-iodo-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



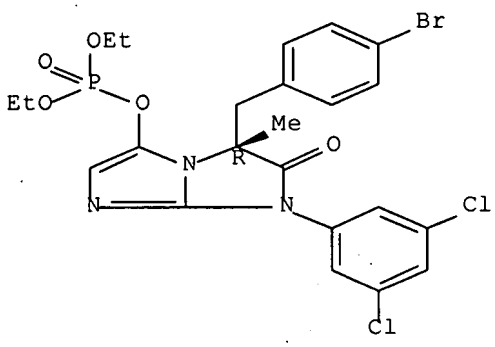
RN 397329-88-3 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



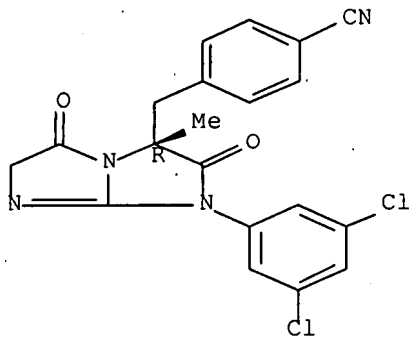
RN 397329-89-4 ZCAPLUS
CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



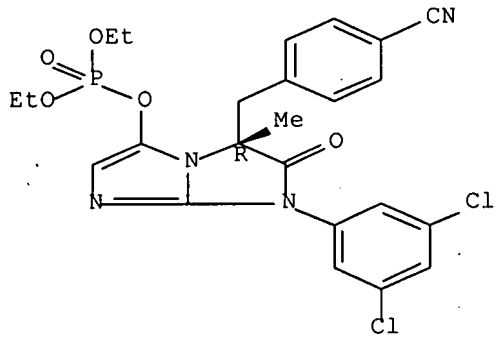
RN 835917-16-3 ZCAPLUS
CN Benzonitrile, 4-[[(3R)-1-(3,5-dichlorophenyl)-2,3,5,6-tetrahydro-3-methyl-2,5-dioxo-1H-imidazo[1,2-a]imidazol-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 835917-17-4 ZCAPLUS
CN Phosphoric acid, (3R)-3-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

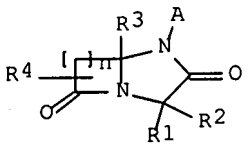
L34 ANSWER 9 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:817893 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:332191
TITLE: Preparation of new bicyclic arylimidazolones with nootropic action
INVENTOR(S): Farina, Carlo; Gagliardi, Stefania; Parini, Carlo; Martinelli, Marisa; Ghelardini, Carla
PATENT ASSIGNEE(S): Nikem Research S.r.l., Italy
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004085438	A2	20041007	WO 2004-EP50339	20040322
WO 2004085438	A3	20041125		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004224087	A1	20041007	AU 2004-224087	20040322
CA 2520008	A1	20041007	CA 2004-2520008	20040322
EP 1608655	A2	20051228	EP 2004-741432	20040322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
BR 2004008601	A	20060307	BR 2004-8601	20040322
CN 1756757	A	20060405	CN 2004-80005591	20040322
JP 2006523198	T	20061012	JP 2006-505479	20040322
NO 2005004898	A	20051024	NO 2005-4898	20051024
IN 2005CN02757	A	20070525	IN 2005-CN2757	20051024
US 2007027137	A1	20070201	US 2006-550483	20060616

PRIORITY APPLN. INFO.: IT 2003-MI573 A 20030324
WO 2004-EP50339 W 20040322

OTHER SOURCE(S): CASREACT 141:332191; MARPAT 141:332191
GI

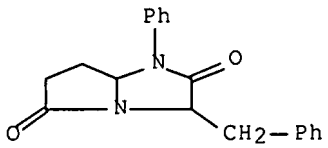


I

AB The title compds. [I; A = aryl, heteroaryl, arylalkyl; R1 = H, arylalkyl, heterocyclylalkyl, etc.; R2 = H, alkyl, arylakyl, Ph; or R1 and R2, taken together, form a saturated carbocyclic ring; R3 = H, alkyl, aryl, arylalkyl, heterocyclyl; n = 2-4; R4 = H, alkyl, aryl, etc.] having nootropic action (i.e., protecting and stimulating cerebral functions), analgesic action and antihyperalgesic action, and therefore useful for the treatment of cognitive deficits, and of various types of pain, were prepared Thus, reacting tetrahydro-pyrrolo[1,2-a]imidazole-2,5-dione with iodobenzene afforded 1-phenyl-tetrahydro-1H-pyrrolo[1,2-a]imidazole-2,5-dione which was evaluated in a rat model of mononeuropathy (data given). The pharmaceutical compns. comprising the compound I are claimed.

IT ***770731-04-9P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrroloimidazolones with nootropic action)
RN 770731-04-9 ZCAPLUS
CN 1H-Pyrrolo[1,2-a]imidazole-2,5(3H,6H)-dione, dihydro-1-phenyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

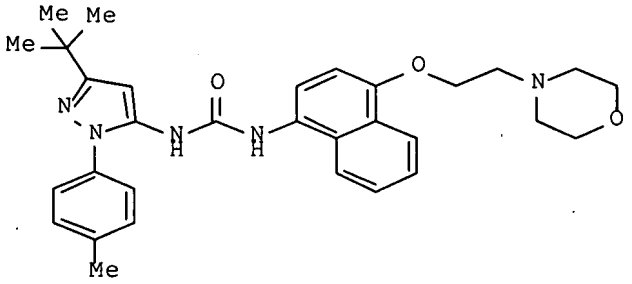


L34 ANSWER 10 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:142968 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:193056
TITLE: Combinations of active agents with p38 MAP kinase inhibitors, pharmaceutical compositions, and use in the treatment of cytokine-mediated diseases
INVENTOR(S): Simianer, Stefan; Bilbault, Pascal; Cappola, Michael L.; Way, Susan Lynn
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim France
SOURCE: PCT Int. Appl., 168 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014387	A1	20040219	WO 2003-US25341	20030812
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004110755	A1	20040610	US 2003-638702	20030811
CA 2497448	A1	20040219	CA 2003-2497448	20030812
AU 2003256410	A1	20040225	AU 2003-256410	20030812
EP 1530477	A1	20050518	EP 2003-785255	20030812
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006501218	T	20060112	JP 2004-528105	20030812
US 2007099832	A1	20070503	US 2006-539376	20061006

PRIORITY APPLN. INFO.:
US 2002-403115P P 20020813
US 2003-638702 B1 20030811
WO 2003-US25341 W 20030812

GI



I

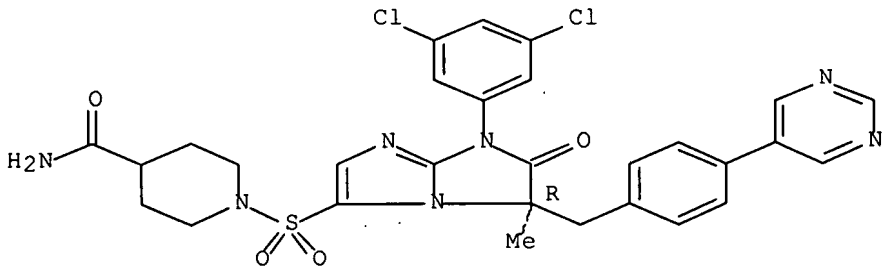
AB The invention relates to pharmaceutical combination therapies based on p38 kinase inhibitors and another active ingredients, pharmaceutical compns. comprising such combinations, processes for preparing them, and their use in the treatment of cytokine-mediated diseases. Preparation of I (BIRB 796 BS) is described.

IT ***321656-57-9***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combinations of active agents with p38 MAP kinase inhibitors, pharmaceutical compns., and use in treatment of cytokine-mediated diseases)

RN 321656-57-9 ZCAPLUS

CN 4-Piperidinecarboxamide, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:597593 ZCAPLUS Full-text
DOCUMENT NUMBER: 139:276851
TITLE: Regiocontrolled synthesis of highly-functionalized fused imidazoles: a novel synthesis of second generation LFA-1 inhibitors
AUTHOR(S): Frutos, Rogelio P.; Johnson, Michael
CORPORATE SOURCE: Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT,

06877-0368, USA
SOURCE: Tetrahedron Letters (2003), 44(34), 6509-6511
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:276851
GI

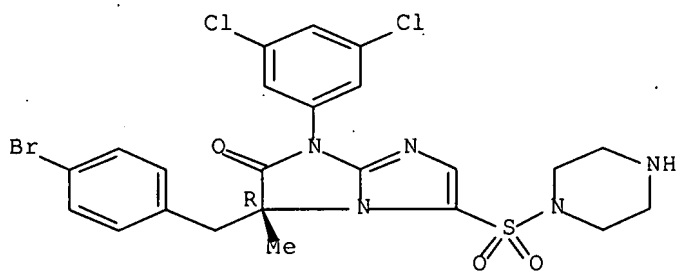
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A new and reliable route to a new class of LFA-1 inhibitors such as I has been developed. A key aspect of this route is the transformation of amino amide II into iodide III in four steps. Iodide III is a key advanced intermediate used in the synthesis of all second-generation 1H-imidazo[1,2-α]imidazol-2-one LFA-1 inhibitors.

IT ***321656-61-5P 321656-73-9P 397329-88-3P 397329-89-4P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regiocontrolled synthesis of fused imidazoles)

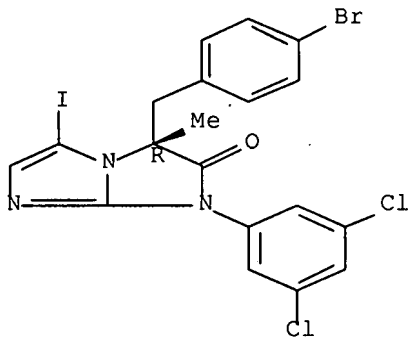
RN 321656-61-5 ZCAPLUS
CN Piperazine, 1-[[(3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



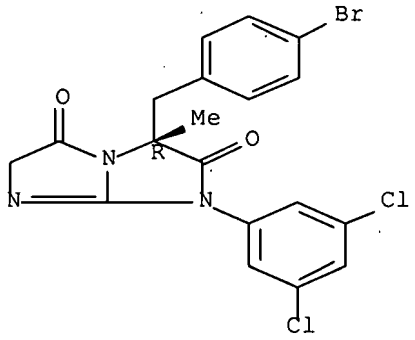
RN 321656-73-9 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



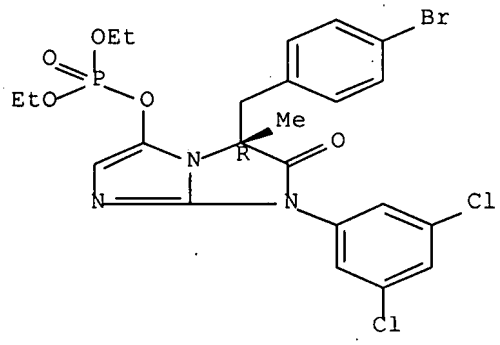
RN 397329-88-3 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



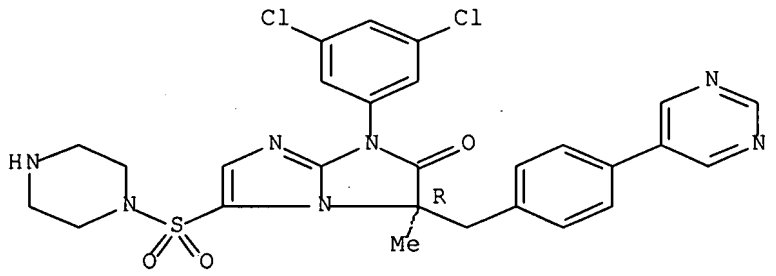
RN 397329-89-4 ZCAPLUS
CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT *321656-63-7P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(regiocontrolled synthesis of fused imidazoles)
RN 321656-63-7 ZCAPLUS
CN Piperazine, 1-[[(3R)-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-3-[[4-(5-pyrimidinyl)phenyl]methyl]-1H-imidazo[1,2-a]imidazol-5-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

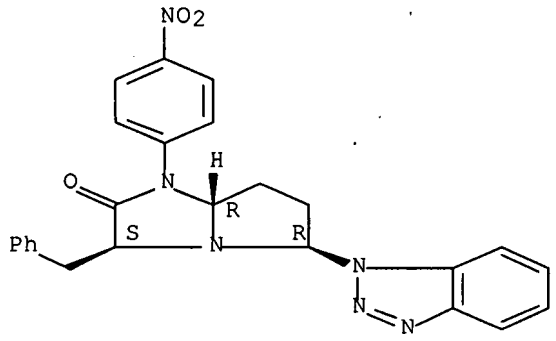


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 12 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:452282 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:169459
TITLE: Syntheses of Optically Active Tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones and Hexahydroimidazo[1,2-a]pyridin-2(3H)-ones
AUTHOR(S): Katritzky, Alan R.; He, Hai-Ying; Wang, Jing
CORPORATE SOURCE: Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: Journal of Organic Chemistry (2002), 67(14), 4951-4956
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:169459
AB The reactions of (2S)-2-amino-2-substituted-N-(4-nitrophenyl)acetamides, succindialdehyde, and benzotriazole afforded enantiopure (3S,5R,7aR)-5-(1H-1,2,3-benzotriazol-1-yl)-3-substituted-1-(4- nitrophenyl)tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones, which were converted by sodium borohydride into (3S,7aR)-3-substituted-1-(4- nitrophenyl)tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones. Chiral (2S)-2-amino-2-substituted-N-(4-methylphenyl)acetamides, easily prepared in two steps from N-Boc-α-amino acids, similarly reacted with glutaraldehyde and benzotriazole to generate 5-benzotriazolyl-3- substituted-hexahydroimidazo[1,2-a]pyridin-2(3H)-ones, which were converted by sodium borohydride directly into optically active 3-substituted-hexahydroimidazo[1,2-a]pyridin-2(3H)-ones.
IT *447462-63-7P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses of optically active tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones and hexahydroimidazo[1,2-a]pyridin-2(3H)-ones)
RN 447462-63-7 ZCAPLUS

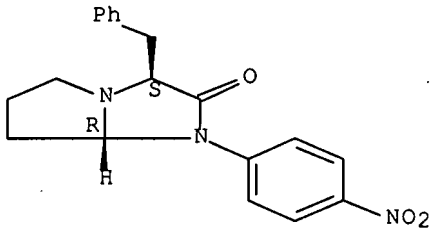
CN 1H-Pyrrolo[1,2-a]imidazol-2(3H)-one, 5-(1H-benzotriazol-1-yl)tetrahydro-1-(4-nitrophenyl)-3-(phenylmethyl)-, (3S,5R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT ***447462-71-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of optically active tetrahydro-1H-pyrrolo[1,2-a]imidazol-2-ones and hexahydroimidazo[1,2-a]pyridin-2(3H)-ones)
RN 447462-71-7 ZCAPLUS
CN 1H-Pyrrolo[1,2-a]imidazol-2(3H)-one, tetrahydro-1-(4-nitrophenyl)-3-(phenylmethyl)-, (3S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 13 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:123008 ZCAPLUS Full-text
DOCUMENT NUMBER: 136:167376
TITLE: Novel preparation of (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one, an intermediate for antiinflammatory agents and immunomodulators
INVENTOR(S): Frutos, Rogelio P.; Johnson, Michael Dale
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012243	A2	20020214	WO 2001-US23996	20010731
WO 2002012243	A3	20020620		
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2416906	A1	20020214	CA 2001-2416906	20010731
US 2002028949	A1	20020307	US 2001-918915	20010731
US 6414161	B2	20020702		
EP 1309595	A2	20030514	EP 2001-957358	20010731
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
JP 2004505978	T	20040226	JP 2002-518218	20010731
US 2002072615	A1	20020613	US 2002-76829	20020215
US 6433183	B2	20020813		
US 2002072610	A1	20020613	US 2002-77045	20020215
US 6441183	B2	20020827		
US 2002082441	A1	20020627	US 2002-77044	20020215
US 6458986	B2	20021001		
US 2002087009	A1	20020704	US 2002-77043	20020215
US 6437148	B2	20020820		
PRIORITY APPLN. INFO.:			US 2000-224166P	P 20000809
			US 2001-918915	A3 20010731
			WO 2001-US23996	W 20010731

OTHER SOURCE(S): CASREACT 136:167376; MARPAT 136:167376
GI

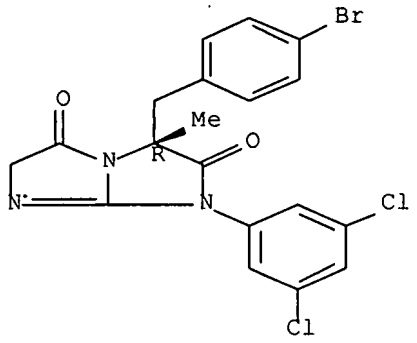
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A novel process for the preparation of (R)-3-(4-bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one I is disclosed. I is useful as an intermediate in the preparation of certain small mols. that are useful in the treatment or prevention of inflammatory and immune cell-mediated diseases. The invention also relates to certain intermediates used in the process. Cyclization of amino amide II with an isocyanatoacetate ester RO2CCH2NCO [R = C1-6 alkyl] using a triarylphosphine, a carbon tetrahalide, and a tertiary amine, gives III. Optional alkaline hydrolysis of the resultant imidazolidinone ester III gives the acid III [R = H]. Cyclization of III [R = C1-6 alkyl] using a Lewis acid and a phosphine oxide, or cyclization of III [R = H] using a coupling agent, gives dione IV. Reaction of IV with a strong base and a chlorophosphate (R'O)2POCl gives an enol phosphate V, which is iodinated with Me3SiI or NaI/Me3SiCl to give I. In a specific example using R = R' = Et, a yield of 89% was obtained in the key cyclization of III (AlMe3 and Ph3PO), and 69% was obtained in the final iodination step (NaI/Me3SiCl).

IT ***397329-88-3P***, (3R)-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-3-methyl-1,6-dihydroimidazo[1,2-a]imidazole-2,5-dione ***397329-89-4P***, Phosphoric acid (3R)-5-(4-bromobenzyl)-7-(3,5-dichlorophenyl)-5-methyl-6-oxo-6,7-dihydro-5H-imidazo[1,2-a]imidazol-3-yl diethyl ester
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-imidazo[1,2-a]imidazol-2-one derivative as intermediate for
immunomodulators and antiinflammatory agents)

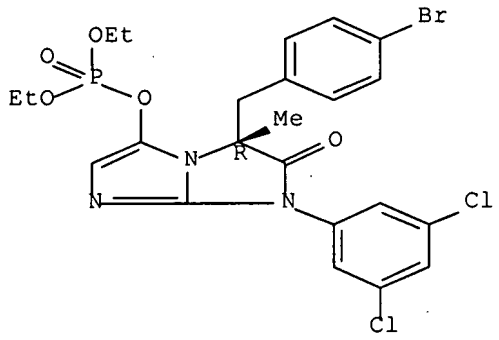
RN 397329-88-3 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazole-2,5(3H,6H)-dione, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



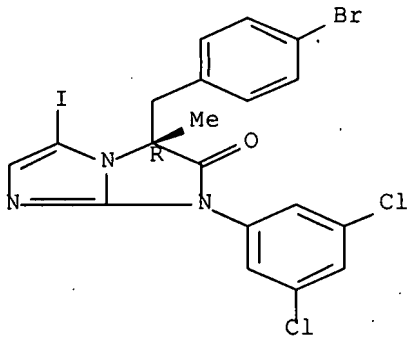
RN 397329-89-4 ZCAPLUS
CN Phosphoric acid, (3R)-3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

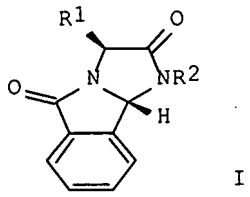


IT ***321656-73-9P***, (3R)-(4-Bromobenzyl)-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-1H-imidazo[1,2-a]imidazol-2-one
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1H-imidazo[1,2-a]imidazol-2-one derivative as intermediate for
immunomodulators and antiinflammatory agents)
RN 321656-73-9 ZCAPLUS
CN 1H-Imidazo[1,2-a]imidazol-2(3H)-one, 3-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-5-iodo-3-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 14 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:541387 ZCAPLUS Full-text
DOCUMENT NUMBER: 135:357878
TITLE: Stereoselective syntheses of 1H-imidazo[2,1-a]isoindole-2,5(3H,9bH)-diones
AUTHOR(S): Katritzky, Alan R.; Xu, Yong-Jiang; He, Hai-Ying; Steel, Peter J.
CORPORATE SOURCE: Center for Heterocyclic Chemistry, Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (15), 1767-1770
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:357878
GI



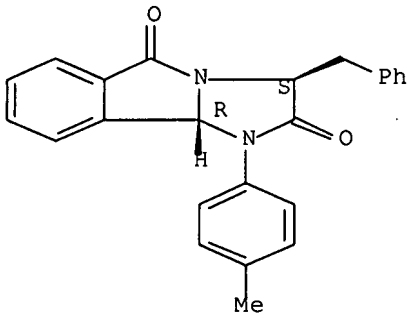
I

AB Title imidazoisoindolediones I (R1 = MeCH2CHMe, Me, Me2CH, benzyl; R2 = 4-MeC6H4, Ph, 4-FC6H4, Bu, cyclohexyl) were prepared in 67-96% yields with high stereoselectivities via intermol. condensation of 2-formylbenzoic acid and α-amino amides R1CH(NH2)CONHR2 in the presence of a catalytic amount of p-toluenesulfonic acid. Intermediate α-amino amides R1CH(NH2)CONHR2 were obtained in two steps from easily available chiral N-Boc-α-amino acids.

IT ***372187-77-4P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure of imidazoisoindoledione prepared via cyclocondensation of formylbenzoic acid with amino acid amides)
RN 372187-77-4 ZCAPLUS

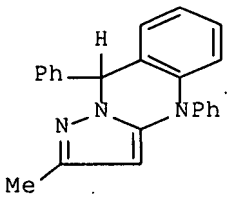
CN 1H-Imidazo[2,1-a]isoindole-2,5(3H,9bH)-dione, 1-(4-methylphenyl)-3-(phenylmethyl)-, (3S,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

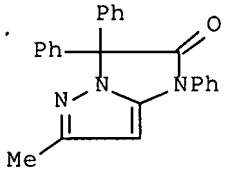


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

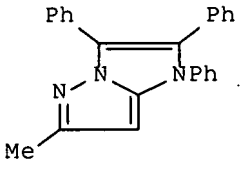
L34 ANSWER 15 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:68049 ZCAPLUS Full-text
DOCUMENT NUMBER: 128:154055
TITLE: Synthesis of pyrazolo-fused heterocycles by a tandem Appel's dehydration/electrocyclization methodology
AUTHOR(S): Lee, Kee-Jung; Kwon, Heung-Taeck; Kim, Boo-Geun
CORPORATE SOURCE: Department of Industrial Chemistry, Hanyang University, Seoul, 133-791, S. Korea
SOURCE: Journal of Heterocyclic Chemistry (1997), 34(6), 1795-1799
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



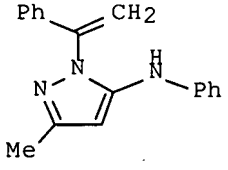
I



II



IV



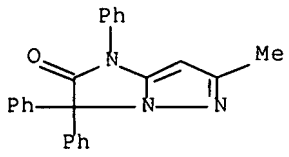
V

AB The hydrazones of benzophenone, benzil, and acetophenone were allowed to react with acetoacetanilide to give azinoamides PhCR:NN:CMeCH2CONHPh (I, R = Ph, COPh, Me), and the reaction of I with Appel's dehydration conditions (triphenylphosphine/carbon tetrachloride/triethylamine) led to the corresponding azinoketimines, which underwent electrocyclic ring closure under the reaction conditions to give pyrazolo-fused heterocycles. Azinoamide I (R = Ph) gave a 4,9-dihydropyrazolo[5,1-b]quinazoline II, while I (R = COPh) yielded 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-one III and 1H-imidazo[1,2-b]pyrazole IV. I (R = Me) gave a monocyclic N-α-styryl-5-(phenylamino)pyrazole V.

IT ***202481-62-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazolo-fused heterocycles by Appel's dehydration/electrocyclization of hydrazones)

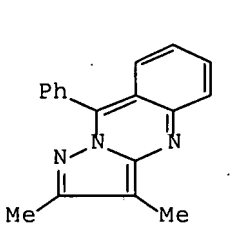
RN 202481-62-7 ZCAPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 16 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:196519 ZCAPLUS Full-text
DOCUMENT NUMBER: 106:196519
TITLE: Reactions of azines. 12. Preparation and reactions of triphenyl[2-([phenyl(methoxycarbonyl)methylene]hydrazono)propyl]phosphonium bromide
AUTHOR(S): Schweizer, E. E.; Hayes, J. E.; Rheingold, A.; Xu, Wei
CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19716, USA
SOURCE: Journal of Organic Chemistry (1987), 52(9), 1810-16
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:196519
GI



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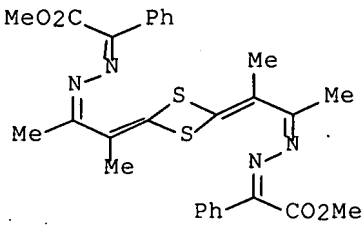
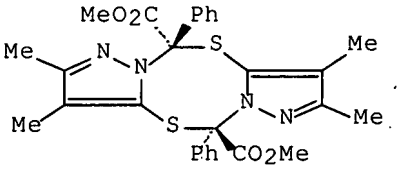


II



III

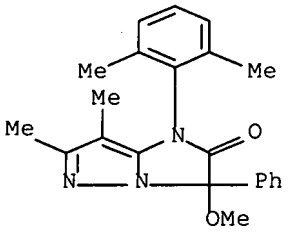
AB Ph(MeO2C)C:NN:CMeCHRP+Ph3 X- (R = H, X = Br; R = Me, X = iodide) and their ylides Ph(MeO2C)C:NN:CMeCR:PPh3 were prepared and their reactions to give, e.g., pyrazoloquinazoline I, desaurine (II), and dipyrazolodiazadithiocine III are described. The crystal structures of I-III were determined

IT ***107769-80-2P 107769-81-3P***

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

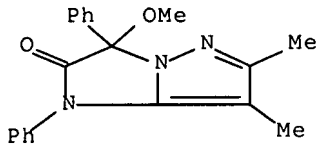
RN 107769-80-2 ZCAPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(2,6-dimethylphenyl)-3-methoxy-6,7-dimethyl-3-phenyl- (9CI) (CA INDEX NAME)



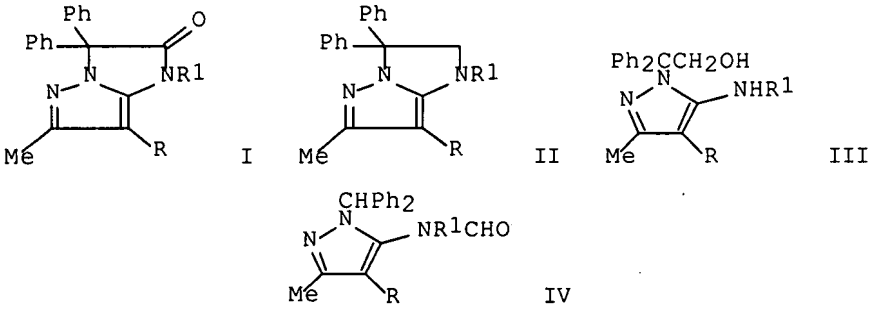
RN 107769-81-3 ZCAPLUS

CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 3-methoxy-6,7-dimethyl-1,3-diphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 17 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN

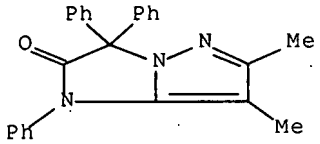
ACCESSION NUMBER: 1985:6313 ZCAPLUS Full-text
DOCUMENT NUMBER: 102:6313
TITLE: Novel lithium aluminum hydride reduction pathway. Reactions of 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-ones with lithium aluminum hydride. Preparations of 2,3-dihydro-1H-imidazo[1,2-b]pyrazoles and side products
AUTHOR(S): Schweizer, Edward E.; Lee, Kee Jung
CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19711, USA
SOURCE: Journal of Organic Chemistry (1984), 49(25), 4848-53
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:6313
GI



AB The direct LiAlH4 reduction of 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-ones (I) to 2,3-dihydro-1H-imidazo[1,2-b]pyrazoles (II) was unsuccessful. Reduction of I (R, R1 = Me, Ph; Et, Ph; Me, 4-MeOC6H4; Et, 4-F3CC6H4) gave an N-carbonyl cleavage followed by carbonyl reduction to amino alcs. III. Reduction of I (R, R1 = Me, Me3C; allyl, Me3C; Me, Me; allyl, Me) gave an unusual formamide product, IV, further LiAlH4 treatment of which gave II. Dehydrative ring closure of compds. III (R = Me, Et; R1 = Ph) with P2O5 gave the corresponding II.

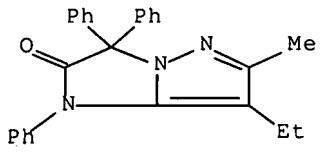
IT ***89726-11-4 89726-13-6 89726-25-0 89726-36-3 92816-79-0***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, with lithium aluminum hydride)

RN 89726-11-4 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)

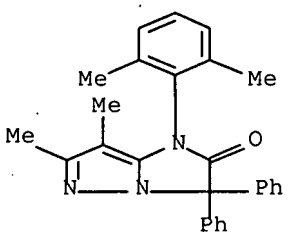


RN 89726-13-6 ZCAPLUS

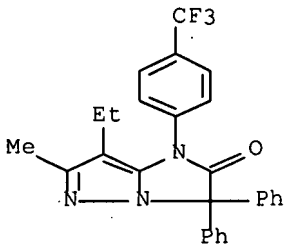
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



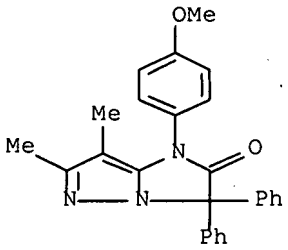
RN 89726-25-0 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(2,6-dimethylphenyl)-6,7-dimethyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



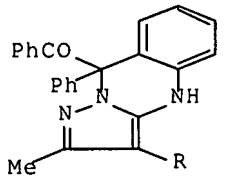
RN 89726-36-3 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-3,3-diphenyl-1-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



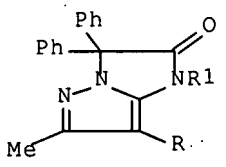
RN 92816-79-0 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(4-methoxyphenyl)-6,7-dimethyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 18 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:209740 ZCAPLUS Full-text
DOCUMENT NUMBER: 100:209740
TITLE: Reactions of azines. 9. Rearrangement of 1-oxo-3,4,8-triaza-2,4,6,7-octatetraenes to 2,3-dihydro-1H-imidazo[1,2-b]pyrazol-2-ones and 4,9-dihydropyrazolo[5,1-b]quinazolines
AUTHOR(S): Schweizer, Edward E.; Lee, Kee Jung
CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19711, USA
SOURCE: Journal of Organic Chemistry (1984), 49(11), 1964-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:209740
GI



III

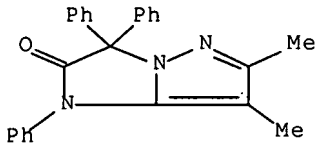


IV

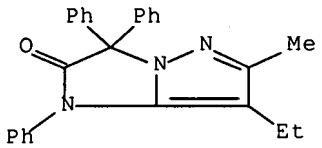
AB The reactions of PhCOCPh:NN:CMeCR:X (I; R = Me, Et, Pr, allyl, PhCH2; X = PPh3) with R1NCO (II; R1 = Me, Me3C, Ph, substituted Ph, etc.) gave the title heterocycles III and IV, presumably via I (X = C:NR1). The III:IV ratio increased with increasing bulk of R and R1 and decreased linearly with increasing σp value of the substituents in II [R1 = (un)substituted phenyl]: ρ = -0.5. The III:IV ratios obtained from I (R = Et) and undistd. II were .apprx.65:35, reversed compared to the results obtained with freshly distilled II.

IT ***89726-11-4P 89726-13-6P 89726-15-8P***
89726-17-0P 89726-18-1P 89726-20-5P
89726-22-7P 89726-24-9P 89726-25-0P
89726-31-8P 89726-33-0P 89726-35-2P
89726-36-3P 89726-37-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

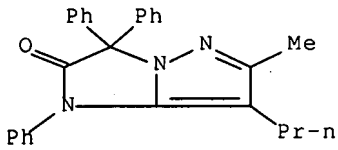
RN 89726-11-4 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



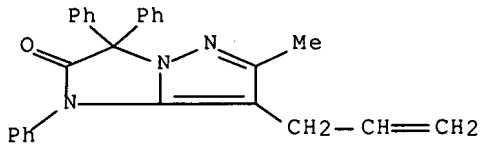
RN 89726-13-6 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



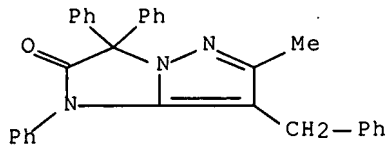
RN 89726-15-8 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl-7-propyl- (9CI) (CA INDEX NAME)



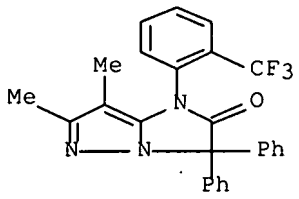
RN 89726-17-0 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl-7-(2-propenyl)- (9CI) (CA INDEX NAME)



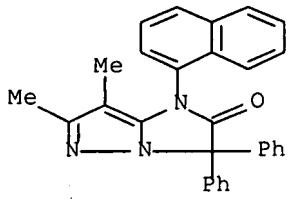
RN 89726-18-1 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6-methyl-1,3,3-triphenyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)



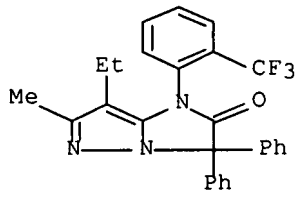
RN 89726-20-5 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-3,3-diphenyl-1-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 89726-22-7 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1-(1-naphthalenyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)

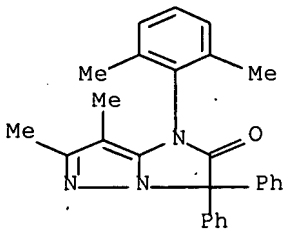


RN 89726-24-9 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-3,3-diphenyl-1-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

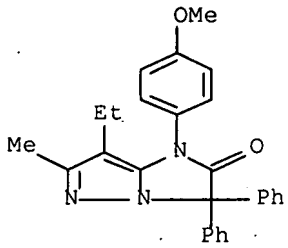


RN 89726-25-0 ZCAPLUS

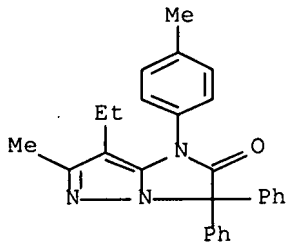
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(2,6-dimethylphenyl)-6,7-dimethyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



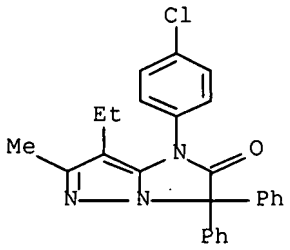
RN 89726-31-8 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-1-(4-methoxyphenyl)-6-methyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



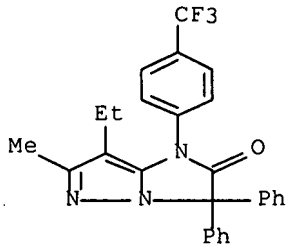
RN 89726-33-0 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1-(4-methylphenyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)



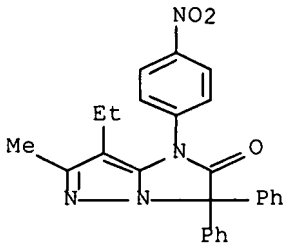
RN 89726-35-2 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 1-(4-chlorophenyl)-7-ethyl-6-methyl-3,3-diphenyl- (9CI) (CA INDEX NAME)



RN 89726-36-3 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-3,3-diphenyl-1-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 89726-37-4 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 7-ethyl-6-methyl-1-(4-nitrophenyl)-3,3-diphenyl- (9CI) (CA INDEX NAME)



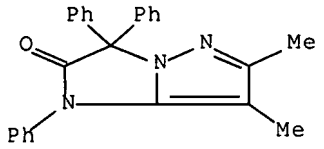
L34 ANSWER 19 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:201300 ZCAPLUS Full-text
DOCUMENT NUMBER: 100:201300
TITLE: The structures of 3-allyl-9-benzoyl-2-methyl-9-phenyl-4,9-dihydropyrazolo[5,1-b]quinazoline, C27H23N3O, and 6,7-dimethyl-1,3,3-triphenyl-1H-imidazo[1,2-b]pyrazol-2(3H)-one, C25H21N3O
AUTHOR(S): Rheingold, A. L.; Fultz, W. C.; Schweizer, E. E.; Lee, K. J.
CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19716, USA
SOURCE: Acta Crystallographica, Section C: Crystal Structure

Communications (1984), C40(4), 687-90
CODEN: ACSCEE; ISSN: 0108-2701
DOCUMENT TYPE: Journal
LANGUAGE: English

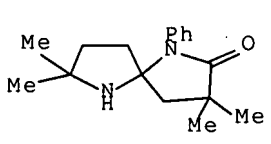
AB C27H23N3O is orthorhombic, space group Pbcs, with a 13.025(4), b 15.99(3)°;, and c 20.593(6) Å at 297 K; d.(calculated) = 1.26 for Z = 8; R for 1671 unique reflections [I ≥ 2σ(I)] = 0.0728, C25H21N3O is, monoclinic, space group P21/c, with a 11.234(4), b 7.021(1), c 25.330(6) Å, and β 91.83(3)° at 299 K; d.(calculated) = 1.26 for Z = 4. R For 1383 unique reflections [I ≥ 2.75 σ (I)] = 0.0770. Atomic parameters are given. Bond distances and angles are all within the expected ranges. The 1,2-diazacyclopentadiene rings in both structures are nearly planar.

IT ***89726-11-4***
RL: PRP (Properties)
(crystal structure of)

RN 89726-11-4 ZCAPLUS
CN 1H-Imidazo[1,2-b]pyrazol-2(3H)-one, 6,7-dimethyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 20 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:22339 ZCAPLUS Full-text
DOCUMENT NUMBER: 92:22339
TITLE: Reactions of ketenimines with nitrones
AUTHOR(S): Tsuge, Otohiko; Watanabe, Hiroyuki; Masuda, Kichiro; Yousif, Mohamed M.
CORPORATE SOURCE: Res. Inst. Ind. Sci., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of Organic Chemistry (1979), 44(25), 4543-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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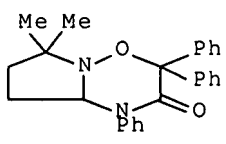
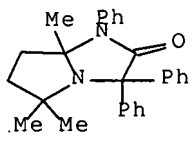


II



III

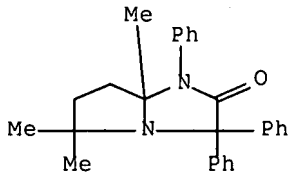
AB Dimethylketene-N-phenylimine reacts with benzylidenaniline N-oxides and cinnamylidenaniline N-oxide to give the corresponding 1:1 adducts, 1-[o-

(benzylidenamino)phenyl]-1,1-dimethylacetanilides, which are easily hydrolyzed to 3,3-dimethyloxindole, whereas the reaction of the ketenimine with cyclic nitrones such as 1-pyrroline 1-oxides afforded 1:1 adducts, imidazolidinone and (or) diazaspiro[4.4]nonanone derivative I. In the reaction of diphenylketene-N-phenylimine with cyclic nitrones, a perhydropyrrooxadiazinone II or imidazolidinone III is formed, depending on the nature of cyclic nitrones.

IT ***71871-89-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71871-89-1 ZCAPLUS

CN 1H-Pyrrolo[1,2-a]imidazol-2(3H)-one, tetrahydro-5,5,7a-trimethyl-1,3,3-triphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 21 OF 21 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:5414 ZCAPLUS Full-text

DOCUMENT NUMBER: 86:5414

TITLE: Synthesis of imidazolino[1,2-f]xanthin-2-ones and their derivatives substituted at the methylene group

AUTHOR(S): Nosachenko, V. I.; Kochergin, P. M.; Steblyuk, P. N.

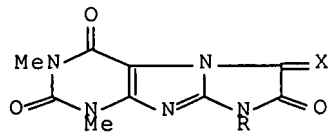
CORPORATE SOURCE: Zaporozh. Med. Inst., Zaporozhe, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1976), (8), 1132-5
CODEN: KGSSAQ; ISSN: 0132-6244

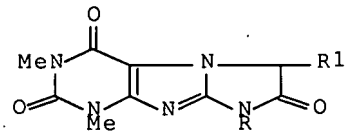
DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



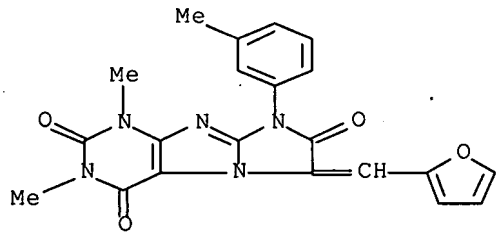
I



II

AB Imidazoloxanthinones (I, R = H, Ph, m-MeC6H4, X = H2) were obtained in 70-80% yields from the appropriate theophylline by treatment with a haloacetate followed by cyclization. Condensation of I with aldehydes and ketones gave 50-94% I (X = PhCH, p-Me2NC6H4CH, PhCH:CHCH, Me2CH, furfurylidene, isatin residue). Addnl. obtained were I (X = p-Me2NC6H4N) and II (R1 = PhN:N, p-H2NSO2C6H4N:N, p-MeOC6H4N:N).

IT *61034-26-2P*
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61034-26-2 ZCAPLUS
CN 1H-Imidazo[2,1-f]purine-2,4,7(3H,6H,8H)-trione, 6-(2-furanylmethylene)-1,3-dimethyl-8-(3-methylphenyl)- (9CI) (CA INDEX NAME)



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L1                STRUCTURE UPLOADED
L2            27 SEA SSS SAM L1
                  D STAT QUE L2

     FILE 'ZCAPLUS' ENTERED AT 10:16:34 ON 27 JUN 2007
L3            12 SEA ABB=ON  PLU=ON  L2
L4         22734 SEA ABB=ON  PLU=ON  WU J?/AU
L5          1187 SEA ABB=ON  PLU=ON  KELLY T?/AU
L6           419 SEA ABB=ON  PLU=ON  LEMIEUX R?/AU
L7          1095 SEA ABB=ON  PLU=ON  GOLDBERG D?/AU
L8             8 SEA ABB=ON  PLU=ON  EMEIGH J?/AU
                  E EMEIGH/AU
L9            21 SEA ABB=ON  PLU=ON  SORCEK R?/AU
L10           16 SEA ABB=ON  PLU=ON  L4 AND (L5 OR L6 OR L7 OR L8 OR L9)
L11           11 SEA ABB=ON  PLU=ON  L5 AND (L6 OR L7 OR L8 OR L9)
L12            2 SEA ABB=ON  PLU=ON  L6 AND (L7 OR L8 OR L9)
L13            2 SEA ABB=ON  PLU=ON  L7 AND (L8 OR L9)
L14            3 SEA ABB=ON  PLU=ON  L8 AND L9
L15           22 SEA ABB=ON  PLU=ON  (L10 OR L11 OR L12 OR L13 OR L14)
L16            4 SEA ABB=ON  PLU=ON  L3 AND (L4 OR L5 OR L6 OR L7 OR L8 OR L9)

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L17           24 SEA ABB=ON  PLU=ON  L2 AND CL>0

     FILE 'ZCAPLUS' ENTERED AT 10:24:52 ON 27 JUN 2007
L18            4 SEA ABB=ON  PLU=ON  L17 AND L16

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L20           28 SEA ABB=ON  PLU=ON  L19

     FILE 'REGISTRY' ENTERED AT 10:27:37 ON 27 JUN 2007
L21            0 SEA ABB=ON  PLU=ON  (L4 OR L5 OR L6 OR L7 OR L8 OR L9) AND L20


     FILE 'ZCAPLUS' ENTERED AT 10:28:41 ON 27 JUN 2007
L22            7 SEA ABB=ON  PLU=ON  (L4 OR L5 OR L6 OR L7 OR L8 OR L9) AND L20

L23           23 SEA ABB=ON  PLU=ON  L15 OR L22

     FILE 'REGISTRY' ENTERED AT 10:29:28 ON 27 JUN 2007

     FILE 'ZCAPLUS' ENTERED AT 10:32:32 ON 27 JUN 2007
L24           21 SEA ABB=ON  PLU=ON  L20 NOT L23
                  D SCA
                  D SCA L22

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L25          284 SEA ABB=ON  PLU=ON  L19 AND CL>1 AND BR>0
L26          210 SEA ABB=ON  PLU=ON  L25 AND N>3
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L27          201 SEA ABB=ON  PLU=ON  L26 AND O>1
L28            0 SEA ABB=ON  PLU=ON  L27 AND NC>1
L29           32 SEA ABB=ON  PLU=ON  L27 AND 3/NRS
                 D SCA
L30          125 SEA ABB=ON  PLU=ON  L27 AND 4/NRS
L31           43 SEA ABB=ON  PLU=ON  L27 AND 5/NRS
L32          200 SEA ABB=ON  PLU=ON  (L29 OR L30 OR L31)
L33            1 SEA ABB=ON  PLU=ON  L27 NOT L32
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     FILE 'ZCAPLUS' ENTERED AT 10:45:59 ON 27 JUN 2007
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L34           21 SEA ABB=ON  PLU=ON  L20 NOT L23
                 D IBIB ABS HITSTR L34 1-21


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   26 JUN 2007  HIGHEST RN 939408-72-7
     DICTIONARY FILE UPDATES:  26 JUN 2007  HIGHEST RN 939408-72-7

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     FILE ZCAPLUS

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FILE LAST UPDATED: 26 Jun 2007 (20070626/ED)

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